- *The following is the preliminary technical program and is subject to change. For the latest program, visit www.aiche.org/annual*

## Preliminary Program

# 2006 AICHE ANNUAL MEETING

## November 12-17, 2006

**San Francisco, California, San Francisco Hilton**

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Annual Meeting, San Francisco, CA

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(Outside the US)

**SUNDAY, 12 NOVEMBER 2006**
***9:00 AM - 12:00 PM***
**Sunday Morning Workshop: Career Planning for Prospective Faculty**
***Hilton San Francisco, Plaza A***
**Sunday Workshop for Faculty: Developing Student Skills in Self-Assessment**
***Hilton San Francisco, Plaza B***

**SUNDAY, 12 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**Tutorial on Fuel Cell Technology**
***Hilton San Francisco, Plaza B***
• Fuel Cell Systems: an Introduction for the Chemical Engineer

**SUNDAY, 12 NOVEMBER 2006**
***1:00 PM - 4:00 PM***
**Sunday Afternoon Workshop: Teaching Safety as Capstone Design**
***Hilton San Francisco, Plaza A***

**SUNDAY, 12 NOVEMBER 2006**
***2:00 PM - 5:00 PM***
**Meet the Faculty Candidates**
***Hilton San Francisco, Imperial A & B***

**SUNDAY, 12 NOVEMBER 2006**
***3:00 PM - 5:30 PM***
**The Future of Chemical Engineering - A Roundtable Discussion with Industrial and Government Leaders**
***Hilton San Francisco, Continental 4+5+6***
• The Future of Chemical Engineering: a Perspective from a Developing Nation: Trinidad & Tobago (West Indies)
• The Future of Chemical Engineering: a Perspective from the Energy Industry (Chevron)
• Chemical Engineering: A Boundaryless Profession
• The Future of Chemical Engineering: a Perspective from the Semiconductor Industry
• The Future of Chemical Engineering: a Perspective from the Minerals Processing Industry
• The Future of Chemical Engineering: a Perspective from Sasol
• Energy Scenario in India
• The Future of Chemical Engineering: a Perspective from the Biotechnology Industry
• Panel Discussion and Questions

**SUNDAY, 12 NOVEMBER 2006**
***6:00 PM - 7:00 PM***
**2006 AIChE Honors Ceremony**
***Hilton San Francisco, Continental 4+5+6***

**MONDAY, 13 NOVEMBER 2006**
***8:30 AM - 11:00 AM***
**(22a) Carbon Nanotubes I: Synthesis**
***Hilton San Francisco, Franciscan D***
• Dendrimer-Templated Fe Nanoparticles for the Growth of Single-Wall Carbon Nanotubes by Plasma-Enhanced CVD
• Controlled Diameter and Density Growth of Multi-walled Carbon Nanotube Arrays by Micelle Patterning Method
• Mechanism of Growth of Vertically-Oriented Single-Walled Carbon Nanotubes on Surface: Topologically Confinement Induced Synchronized Alignment and Growth
• Controlling the Morphology of Carbon Nanotube Films by Varying the Area Density of Catalyst Nanoclusters Using Block Copolymer Micellar Thin Films
• Effects of Water on Synthesis of Single-Walled Carbon Nanotubes

**(22b) Bionanotechnology I: Plenary Session**
***Hilton San Francisco, Grand Ballroom A***
• Nanotechnology in Cancer Therapeutics and Diagnostics
• Molecular Evolution of New Viruses for Gene Delivery
• Isolation and Concentration of Biomarkers Using Self-Assembled Nanomaterials

**Adsorption Processes for Water Decontamination**
***Hilton San Francisco, Union Square 21***
• Synthesis of Manganese Oxide Coatings for Adsorption of Trace Metals from Ground Water
• Impacts of Ozonation on the Surface and Adsorption Characteristics of Activated Carbon
• Adsorption of Arsenate on Course Loamy Mixed Hyperthermic Fluventic Haplustept Soil of Punjab, North-West India
• Case Study: the Coagulation Filtration Process for Groundwater Arsenic Removal
• Removal of Estrone from Water with Adsorption on Zeolites Followed by UV Photolysis
• Adsorption and Decontamination of Chemical and Biological Substances in Drinking Water Distribution Systems
• Competitive Adsorption Behavior on the Removal of Iron and Lead from Solution

**Advanced Oxidation Processes & Chemistries for Environmental Applications**
***Hilton San Francisco, Union Square 13***
• Multiple Oxidant Synergism in Chromium Separation from Hanford High Level Nuclear Waste Components
• Oxidative Processes for Treating High-Level Waste Sludge
• A Critical Review of Integrated Advanced Oxidation Processes: Assessment of Process Synergism
• Defense Waste Processing Facility Flowsheet Studies with Simulants to Determine Solvent Build-up in Continuous Runs
• Destruction of Tetraphenylborate Via Wet Air Oxidation Technology

**Advances and Case Studies in Crystallization and Post-Crystallization Processing - I**
***Hilton San Francisco, Lombard***
• The Application of CFD to the Multi-Scale Characterization of Anti-Solvent Addition Crystallization
• Crystal Form Generation of Pharmaceutical Materials Using Nano-Engineered Substrates
• Impurity Management in Integrated Crystallization Systems
• Investigation of Simultaneous Preferential Crystallization for Enantioseparation
• Particle Engineering by Means of Optimal Seeding and Constant-Supersaturation Operation in Anti-Solvent Crystallization
• On-Line Estimation of Diastereometric Resolution with the Use of FBRM, Raman Spectroscopy, and ATR-FTIR
• Assessing the Reliability of Crystal Size Distribution Measurements Obtained by in Situ Video Microscopy and Image Analysis

**Advances in Animal and Plant Cell Culture**
***Hilton San Francisco, Continental 9***
• Engineering Mammalian Host Cell Lines for Reduced Expression of Lactate Dehydrogenase
• Full Process Characterization of Hematopoietic Stem Cell Cultures Using Design of Experiments to Study Individualistic and Interactive Effects of Culture Parameters
• Co-Expression of the Anti-Apoptotic Genes Aven and E1b-19k Improves BHK Cell Performance in Batch and Continuous Perfusion Cultures
• Chromatin Association of Transgenes Regulates the Transcription of Monoclonal Antibodies in DHFR-Amplified CHO Cells
• Biosynthesis of Astaxanthin in Haematococcus Pluvialis under Zinc, Copper and Iron Metal Stresses
• Effects of Arabidopsis ICK1-Mediated Cell-Cycle Arrest on the Physiology and Recombinant Protein Production in Tobacco Cell Suspension Cultures
• A Comparative Study of Mrna Level, Protein Expression and Metabolite Production in Eschscholtzia Californica with Methyl Jasmonate, Salicylic Acid and Their Combination
• Key Enzyme Activities and Anthocyanin Production Instability in Grape Cell Culture

**Advances in Optimization I**
***Hilton San Francisco, Continental 2***
• Tight Convex Underestimators for Arbitrary $C^2$-Continuous Functions
• A Lagrangean Based Branch-and-Cut Technique for Global Optimization of MINLP Problems with Decomposable Structures
• Global Solution of Bilevel Programs with Nonconvex Functions
• Interior-Point Decomposition Approaches for Parallel Solution of Large-Scale Nonlinear Parameter Estimation Problems
• Interior Point Solution of Integrated Plant and Control Design Problems with Embedded MPC
• Degree-of-Freedom-Based Methods for Phasing Centrosymmetric Structures from X-Ray Diffraction Data

**AES Plenary Session**
***Hilton San Francisco, Yosemite A***
• Nanofluidics and Mass-Limited Chemical Analysis: Nanocapillary Array Membranes as Switchable Fluidic Elements for Multidimensional Analyses
• Integrated Microfluidic and Electrasense Microarray Biochips for DNA Analysis
• Ultra-Fast Molecule Sorting and Delivery by Atomic Force Microscopy
• Automated Computational Analysis of Molecular Evolution: Mitochondrial ATP Synthase in Primates and Other Mammals

**Approaches for Non-Viral Gene Delivery**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Engineering Cellular Niches to Regulate Non-Viral Gene Delivery
• Incorporation of Polyethylene Glycol into Self-Assembled Monolayers Enhances Substrate-Mediated Gene Delivery by Nonspecifically- Bound Complexes
• Engineering Aptamer and SIRNA Based Drug Delivery Systems Using Polyelectrolyte Multilayer Films
• Ternary Particles for Sustained Gene Delivery
• Design and Characterization of Targeted Nanoparticles for Systemic Gene Delivery
• Micelleplexes: Terpolymer Micelle-Based Gene Delivery Vectors with Superior DNA Protection against Enzymatic Degradation
• A Modified Polyethylenimine for Light-Triggered DNA Release
• Ferrocene-Containing Cationic Lipids for Gene Delivery: Oxidation State Determines Transfection Activity

**Biomaterials I**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Viscoelastic Properties of Crosslinked Protein Polymer Hydrogels
• Combinatorial Biosurface Chips for Quantitative Characterization of Polymer - Cell Interactions
• Polyelectrolyte Multilayer Assembly of Elastin-like Polymer Conjugates for Creating Multilayered Cellular Architectures
• Electrospun Polyurethanes and Bone Marrow Stromal Cells for Ligament Tissue Engineering
• Producing Shape-Specific Scaffolds for T M J Tissue Engineering Utilizing Dense-Phase $Co_2$
• Polyelectrolyte Multilayer Films for Cell Contacting Applications
• Photopolymerizable Tough Elastomeric Biomaterials
• Multilayered Polymer Thin Films for Sequential Delivery of Multiple Agents

**Characterization of Engineered Particles and Nano-Structured Particles**
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Mechanical Properties of Nanoparticle Chain

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Aggregates by Combined AFM and SEM: Isolated Aggregates and Networks
• The Evolution of Branching during Flame Growth of Silica Aggregates
• Surface Composition- and Structure-Dependent Optical Properties of InGaP Nanoparticles
• Characterization of Cobalt-Substituted Ferrite Nanoparticles for Use in Sensors
• Photo-Assisted Dissolution of SiB Nanocrystal
• A Quantitative Method for Reconstructing Blend Composition Distributions in the Presence of Agglomerates

**Chemical Engineering in the First Year**
***Hilton San Francisco, Van Ness***
• Using Sneakers to Step into Chemical Engineering
• Fuel Cell Car Performance Design Project in a Freshman Introduction to Engineering Course
• Chemical Engineering Laboratory Exercises with Design Problems for First Year Engineering Students
• Lab-on-a-Chip Design/Build Project in a First-Year Engineering Course
• High School and First Year College Process and Product Design Experiences with Slime
• Project-Based Learning in a First-Year Chemical Engineering Course
• Design of a Freshman Chemical Engineering Course
• Using Lego Mindstorms for Introducing Freshmen to Chemical Engineering

**Educational Software Demonstrations**
***Hilton San Francisco, Grand Ballroom B***
• Distributed Dynamic Simulation of Water Process Plants for Collaborative Learning
• Real Labs at a Distance
• Superpro Designer: an Interactive Software Tool for Designing and Evaluating Integrated Chemical, Biochemical, and Environmental Processes
• A Web-Based Tool to Support Learning Engineering and Problem Solving
• Polymath 6.1 – Now Supports Problem Solving in Excel and Matlab
• Interactive Simulation for Teaching Engineering Economics

**Environmental Applications of Adsorption I**
***Hilton San Francisco, Sutter***
• Donnan Principle Based Hybrid Nanosorbents for Selective Environmental Separation
• Polymeric Chelating-Adsorbents and Their Use in the Adsorption of Arsenic Ions from Aqueous Solutions
• Using Nitrogen and Carbon Dioxide Adsorption to Estimate Arsenic(V) Bioaccessibility in Soils
• Adsorption of *Bacillus Subtilus* on Carbon Nanotubes and Other Porous Media
• Treatment of Cu-CMP Waste Streams Containing Copper (II) Using Polyethylenimine (Pei)
• Adsorption of Chromium(VI) from Aqueous Solution on a Surfactant Modified Zeolite
• Process Analysis of Biosorption Kinetics of Heavy Metal Ions

**Extractive Separations**
***Hilton San Francisco, Mason***
• Novel Solvents for Extractive Separations
• Extractive Catalyst Recovery in an Ionic Liquid Process for 2,5-Dihydrofuran
• Novel Solvent-Resistant Hydrophilic Hollow Fiber Membranes for Membrane Solvent Back Extraction
• Centrifugal Extractors/Separators - Scaling up from Lab Scale to Full Production Size Units
• High-Performance Tray Technology Enhances Extraction
• Design Practice for Packed Liquid Liquid Extraction Columns

**Fundamentals of Adsorption and Ion Exchange I**
***Hilton San Francisco, Powell***
• Adsorption of *n*-Alkanes on 5a Measured Using the ZLC Method
• Characterization of the Microporosity in Mesoporous Adsorbents by Hydrocarbon Adsorption
• Experimental and Theoretical Studies of the Relaxation Processes Associated with Adsorption/Desorption Hysteresis in Mesoporous Materials
• Evidence of Single-File Diffusion by Tracer Zero Length Column Method
• A Generalized Ono-Kondo Lattice Model for High-
• Thermodynamic Approach to Adsorption Deformation
• A Note on Protein Aggregation from Aqueous Solution

**Fundamentals of Protein Degradation and Stabilization**
***Hilton San Francisco, Union Square 1 & 2***
• Self-Assembly, Phase Separation, and Unfolding of Coarse-Grained Proteins in Solution
• Computer Simulation of Fibril Forming Peptides with an Intermediate Resolution Protein Model
• Computing Free Energies of Peptide-Mediated Protein-Protein Interactions in Modeling Immune System Response
• Impact of Ion Hydration and Preferential Interactions on Salt-Induced Protein Deactivation Kinetics
• Thermodynamics, Structure, and Oligomerization States of Key Intermediates in Non-Native Chymotrypsinogen Aggregate Initiation and Growth
• Structural Studies of the Self-Assembly and Stability of Viral Capsids

**High Throughput Biotechnologies**
***Hilton San Francisco, Continental 7***
• Large DNA Synthesis on a Chip with Oligonucleotide Mixtures by Solid Phase Pcr and Ligation Chain Reaction
• High Throughput Screening of Kinases with Ruthenium Inhibitors
• Large-Scale Proteomic Analysis of Human Urinary Exosomes
• Parallel Peptide Synthesis on Microfluidic Microarrays for Epitope Mapping and Cell Adhesion Assays
• High Throughput Genomic Analysis Using Maldi-TOF MS and Solid-Phase Capturable Dideoxynucleotides
• Production of Aromatic Compounds by Metabolic Engineering
• Application of Quadrupole Magnetic Sorter (QMS) in T-Cell and Alloreactive T-Cell Depletions for Mismatched Bone Marrow Transplants
• Functional Genomics Approach to the Identification of Genes Encoding Substrates of the Twin-Arginine Translocation Pathway
• Production of Citric Acid from a Novel Substrate (Mahua Flower) by Using *Aspergillus* Niger MTCC 282

**In Honor of Larry Tavlarides on His 65th Birthday**
***Hilton San Francisco, Union Square 19 & 20***
• A Review of Larry's Contributions to Liquid-Liquid Systems
• Simulation of Drop Breakage in a Turbulent Pipe Flow with Computational Fluid Dynamics and Population Balances Via Operator Methods
• Effects of Charge Discreteness on Electrostatic Interparticle Interactions in Colloidal Dispersions
• A Criterion for "Coffee-Ring" Formation
• Defining Mixing
• Effect of Impeller Geometry, Physical Properties and Process Parameters on Foam Formation in a Continuous Mechanical Whipper
• Novel Fluid-Particle Interaction Mechanisms in Dispersions

**Interfacial Phenomena Plenary Session**
***Hilton San Francisco, Union Square 22***
• Synthetic Protein-Mimicking Materials
• Thin Colloidal Films: Applications to Concentrated Suspensions, Foams and Emulsions
• States of Colloidal Aggregation: Progress and Challenges

**Ionic Liquids: Thermodynamics and Transport**
***Hilton San Francisco, Union Square 5 & 6***
• Separation Science with Ionic Liquids
• Prediction of Binary Vapor-Liquid Equilibria for Hydrofluorocarbons and Imidazolium Based Ionic Liquid Systems Using Cosmo-RS
• Thermodynamic and Transport Characteristics of $Co_2$ in Ionic Liquids
• Design and Applications of Ionic Liquids for Electrochemical Systems
• Volatility of Room-Temperature Ionic Liquids: Distilling the Undistillable
• Using Surface Free Energy to Predict Gas Solubility in Imidazolium-, Phosphonium-, and Ammonium-Based Room Temperature Ionic Liquids
• Modeling Carbon Dioxide - Imidazolium-Based Ionic -Liquid Phase Equilibria with the TPC-PSAFT Equation of State
• Structure and Transport in Pyrrolidinium- and Imidazolium- TFSI Ionic Liquids Doped with LiTFSI
• Understanding the Role of Dissolved Water on the Properties of Ionic Liquids: an Atomistic Simulation Study

**Management of Projects and Project Risks**
***Hilton San Francisco, Imperial B***
• Risk Mitigation When Using Accelerated Schedules on Capital Projects
• Managing Projects in Government Restricted Economies
• Project Risk Prevalent in the USA - Placeholder
• Panel Discussion - Developing Project Managers
• "Keeping Project Management on the Success Track"
• A New Generic Knowledge Representation Model for HAZOP Analysis of Chemical Processes
• Concluding Remarks
• Effectively Managing Project Risk and Uncertainty Using Lean Methods
• Growth and Risk Management in Today's Market from the Perspective of an Upstart Engineering Company
• Screening and Review of Off-the-Shelf Discrete Event Simulation Packages from an Integrating Perspective

**Materials Synthesis and Processing with near and Supercritical Fluids I**
***Hilton San Francisco, Union Square 3 & 4***
• Visualization of Spray Characteristics and Resulting Particles in SCF at Different Solute and Solvent Miscibilities
• Powderization of Polymer Solutions by PGSS-Drying Process
• Micro Particles Filled with Liquid Using the Particles from Gas Saturated Solutions Technology
• Copper Chelation Kinetics in Supercritical Carbon Dioxide
• Photoresist Development in Supercritical Carbon Dioxide and a Carbon Dioxide Compatible Salt: Dissolution Kinetics and Swelling Behavior
• Phase Behavior of the Tri-Tertiary-Butyl Benzene– Supercritical Carbon Dioxide System

**Membrane Session Honoring Professor Ed Ma - I**
***Hilton San Francisco, Yosemite C***
• Mixed-Conducting Metal Oxide Materials–from Membrane to Adsorption
• Carbon Dioxide-Selective Membranes for Hydrogen Purification with Water Gas Shift Reaction
• Microporous Layered Silicates for Nanocomposite Membranes
• Pervaporation through Microporous Membranes
• Developments in Proton Conducting Membranes for Hydrogen Separation and Fuel Cell Applications
• Oxygen Separation Using Mixed Ionic-Electronic Conducting Perovskite Membranes: Present and Prospects


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**Membrane Tutorial I**
***Hilton San Francisco, Yosemite B***
• High Performance Tangential Flow Filtration for Bioprocessing Separations
• Membrane Development for the Production of Biopharmaceuticals
• Barrier Membranes for Packaging

**Modeling and Scale-up of Particle Processing**
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Breakup of Nanoparticle Agglomerates Using an in-Line Rotor-Stator- Part II Validated CFD Results
• Nanotechnology at Degussa - from Ideas to Actual Business
• Modeling the Combustion Synthesis of Titania Nanoparticles
• Design and Scale-up of Chemical Reactors for Nanoparticle Precipitation
• Modeling for Filtration
• Breakup of Nanoparticle Clusters Using an in-Line Rotor-Stator
• Residence Time Distribution Studies in a Fluidized Bed of Fumed Silica Nanopowder

**Multiscale Systems Biology**
***Hilton San Francisco, Continental 1***
• A Multiscale Model for Cytoskeletal Mechanics
• Multiscale Simulation of Breast Cancer Tumorigensis Using Single Cell Models and Kinetic Monte Carlo
• Integration of Signal Transduction in Wound Invasion
• Infectious Disease Engineering, Analysis and Simulation of *Leishmania Major*, a Pathogenic Trypanosomatid
• Integrated Modeling of Angiotensin II-Induced Neuronal Plasticity in the Brain
• Signal Dynamics in Sonic Hedgehog Tissue Patterning
• Exploring Biosynthetic Control in Lipid Metabolism
• Systematically Bridging Transcriptional Regulation and Metabolic Phenotype

**Nanofabrication and Nanoscale Processing**
***Hilton San Francisco, California Room***
• Nanotexturing of Glass Surfaces through Controlled Silane Chemistry and Silica Deposition
• Novel Solid-Phase Synthesis of Oligosiloxane Nanostructure Macromolecules
• Nanomanufacturing Via Laser-Induced Hydrodynamic Instabilities in Metal Films
• Particle Integration across Scales Using Self-Assembly and Transfer
• Mediating Fluidic Self-Assembly with Optical Traps
• Optically-Stimulated Surface Diffusion Exploited for Directed Self-Assembly on Amorphous Semiconductors
• Electric Field Driven Assembly and Temperature Dependent Conduction through Nanoparticle-Molecule-Nanoparticle Structures

**Nanomaterials and Devices for Energy Applications**
***Hilton San Francisco, Franciscan A***
• A General Approach Towards Hierarchical Carbon Particles
• Titania Nanotubes as Templates for the Solar Production of Hydrogen
• Effect of Hydrophilic Layer Property on the Activity of Pulse Deposited Pt Catalyst in PEM Fuel Cells
• Nanostructures for Micro and Miniature Fuel Cells by Template Wetting
• Fabrication of Chalcogenide Nanowire Thin Films for Solid State Energy Conversion
• Surface-Mediated Growth of Oriented and Well-Defined Nanocrystalline Anatase Titania Films
• Nano Energetics for Us Navy Percussion Primer Applications

**Nanoscale Thermal Transport**
***Hilton San Francisco, Union Square 23***
• Thermal Conductivity Measurements in Nanofluids
• Heat Transfer in Quasi-One-Dimensional Nanostructures: Effects of Nonlinear Lattice Vibration Modes
• Thermal Resistance of Nanoscopic Liquid-Liquid Interfaces: Dependence on Chemistry and Molecular Architecture
• Interfacial Heat Transfer in Presence of Shear Flow
• Thermal Transport Properties of Nanoporous MFI Zeolite Films: Experiments and Molecular Dynamics Simulation
• Modeling of Ultra-Short Laser Heating of Nanoscale Thin Metal Films Via Coupled Lattice Boltzmann Method
• Nanoscale Thermal Dissipation and Heat Transport by Continuous Wave Laser Induction of Localized Surface Plasmon Resonance in Gold Nanoparticles

**National Student Paper Competition**
***Hilton San Francisco, Taylor***
• Welcoming Remarks
• Modeling Nitrogen Oxide Emissions from Coke Calcining Process
• Verifying Steady-State Assumptions in Laboratory Microdialysis
• Utilization of Wine Waste as a Biofuel
• Characterization of Parameters for Self-Calibration of a Whole-Cell Bacterial Biosensor
• Modeling of Solid Rocket Propellants
• Fabrication of 3D- Tissue Scaffolds in Tissue Engineering
• Dielectrophoresis Based Micro-Devices for Separation and Analysis of Micro-Particles
• Extending Relief for Allergic Conjunctivitis Via Therapeutic Contact Lenses Based on Configurational Biomimetic Imprinting
• Dynamic Surface Tension
• Isolation and Characterization of Insect Cells with Inactive Mitochondria
• Test of How the System Works
• The Viscoelasticity of Thin Film Polymers: An Analysis of Hole Growth
• Novel Polyanhydrides for the Stabilization and Controlled Release of Therapeutic Proteins
• Statistical Process Control for Monitoring *E. Coli* O157:H7 in the U.S. Ground Beef Industry from a Regulatory Standpoint
• Overexpression of Transhydrogenase Enzymes in *E. Coli* to Improve Whole-Cell Biocatalysis
• Acoustic Detection of Failure Modes in Filled Polymer Composites
• Winning Paper of the Southern Region
• Dynamic Surface Tension Winning Paper
Winning Paper of the Western Region Competition

**New Process Patents Class**
***Hilton San Francisco, Union Square 24***
• Considerations in Drafting Chemical Process Patent Applications

**Novel Flows**
***Hilton San Francisco, Union Square 15 & 16***
• Sustainability and Fluid Mechanics
• Integrated Numerical Simulation of Complex Turbulent Flows
• Building a Better Snail: Rheology, Optimization and Gastropod Locomotion
• Shear Thickening Colloidal Dispersions, Flow Jamming at High Stresses & Applications in Ballistic, Stab & Puncture Threat Mitigation
• Some Tools in the Microfluidic Toolbox: (I) Colloidal Shells, (II) a Differential Manometer, (III) an Approach to Sensing Chemical Influences on Cells

**Plenary Session I on Membranes and Bioseparations Honoring Professor Ed Lightfoot**
***Hilton San Francisco, Continental 5***
• Transport Phenomena in Viral-Vectored Vaccines and Genome Sequencing
• Membranes, Phase Interfaces and Separations: Novel Techniques and Membranes — An Overview
• Membrane Processes in the Biotechnology Industry
• Correlation of Protein–Protein Cross Interactions with Separations Behavior

**Plenary Session I: Us-Japan Joint Topical Conference on Medical Engineering, Drug Delivery Systems and Therapeutic Systems**
***Hilton San Francisco, Continental 4***
• Design and Applications of Responsive Polymers in Diagnostics, Separations, Bioprocesses, and Drug Delivery
• Advanced Nanobiomedical Application of the Phosphorylcholine-Polymer Surface Technology (PCST)

**Processing of Nanocomposites**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• An Investigation of Polymeric Nanocomposite: Surface Functionalization and Nanofiller Effect
• Deagglomeration and Mixing of Nanoparticles
• Preparation of Structured Polymer Composites Using an Ultrasonic Focusing Technique
• Flow-Induced Orientation in an Exfoliated Polystyrene/Clay Nanocomposite
• Using SC-$CO_2$ as a Processing Aid for Improving the Properties of Polymer Nanocomposites
• Plasma and Silane Treatment for the Improvement of Polymer-Polymer Interfaces in Nanocomposites
• Swelling and Transport Properties of Epoxy-Amine Gels with Nanoscopic Morphologies

**Reaction Engineering Symposium in Memory of E.E. Petersen**
***Hilton San Francisco, Imperial A***
• Kinetic Modeling of Processes and the Effect of Catalyst Deactivation by Coke Formation
• Block Copolymers Via Controlled Radical Polymerization
• Kinetics and Mechanism of Moisture Interaction with Dielectric Oxides
• Early Single Crystal Work of E.E. Petersen and G. Somorjai and Current Studies on Operando Spectroscopy
• Surface Chemistry and the Single Pellet Diffusion Reactor
• The Effects of Transport and Intrapellet Liquids on Fischer-Tropsch Synthesis Rate and Selectivity
• Validation of Reaction Mechanisms Used to Represent Reaction Kinetics for Catalyzed Processes

**Reaction Kinetics in Electronic Materials Processing**
***Hilton San Francisco, Franciscan B***
• Decomposition Kinetics of Dimethylcadmium by *in-Situ* Raman Spectroscopy and Quantum Chemical Calculations
• Investigation of CdS Thin Film Deposition Kinetics Using a Continuous Flow Microreactor
• Prediction of Reaction Kinetics in ALD of Metal Oxides and Nitrides
• Calculations of the Initial Reaction Mechanisms for $Tio_2$ Atomic Layer Deposition Onto $Sio_2$ Surfaces
• Growth of Epitaxial-$Al_2O_3$ Films on 4 H-Silicon Carbide
• Controlling Ultrashallow Junction Formation through Surface Chemistry

**Separation Engineering for Sustainable Processes**
***Hilton San Francisco, Continental 3***
• Selective Recovery of Ethanol from Water by Pervaporation: Zeolite-Silicone Rubber Mixed Matrix Membranes
• Hydrogen-Permeable Metal Membrane for Highly Efficient Catalytic Reformer
• Membrane Distillation of Ammonia-Containing Wastewater and Utilization of Recovered Ammonia
• Adsorption of Heavy Metal Ions from Squid Oil by Chelate Ion Exchanger
• Equilibria for Adsorption of Heavy Metal Ions on Chi-

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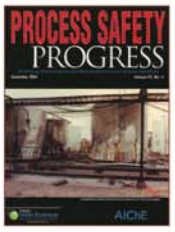
### Process Safety Progress




A quarterly publication, that provides practical process safety information for engineering professionals in the CPI and related industries. Its focus is on chemical and hydrocarbon process safety, loss prevention, and health.

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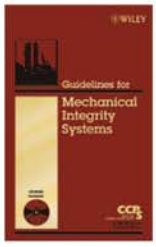



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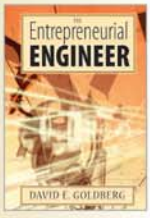


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• Initiator System for Encapsulation of Mesenchymal Stem Cells and Analysis of Osteoblastic Differentiation for Orbital Bone Repair

**Transport Processes in Multiphase Systems I**
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• Keynote Lecture: Experiments and Computation in Multiphase Flow: Rivals or Friends?
• Local Instrumentation for the Investigation of Multiphase Parameters in a Packed Bed
• Detection of Gas-Phase Species by a Microfluidic SERS Apparatus
• Effect of Temperature on Oil Recovery from Oil-Wet Carbonate Reservoirs by Surfactant Brine Imbibition
• Experimental and Theoretical Investigation of Paraffinic Oil Gel Breaking Mechanism
• Keynote Lecture: Computational Methods Employed in Engineering Simulation Software for Multiphase Applications in Industry
• Lattice-Boltzmann Phase-Field Modeling of Multiphase Flows Including Phase Change
• Numerical Simulation of Hydrate Dissociation in Porous Media

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• Scaling Two Phase Batch and Semi-Batch Chemical Processes from Laboratory Scale to Commercial Scale
• Development of an Adsorption Model Using Aspen Custom Modeler as a Troubleshooting and Optimization Tool for Plant Processes

**MONDAY, 13 NOVEMBER 2006**
***11:15 AM - 12:15 PM***
**The Danckwerts Lecture**
***Hilton San Francisco, Grand Ballroom A***
• Hierarchical Modeling of Polymeric Materials

**MONDAY, 13 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**(22a) Carbon Nanotubes II: Characterization, Functionalization and Applications**
***Hilton San Francisco, Franciscan D***
• Dynamics of Single-Walled Carbon Nanotubes in Water
• Functionalization of Carbon Nanotubes Via Supercritical Fluid Treatment
• Functionalization of Carbon Nanotubes by Argon Plasma Assisted Uv Grafting of 1-Vinylimidazole
• Separation of Functionalized Single-Walled Carbon Nanotubes from Non-Functionalized Using a Novel Electro-Diffusion Mechanism
• Tailoring of Pore Structure of Carbon Nanotube Fibers for Biomedical Applications
• Isotropic-Nematic Phase Transition of Single-Walled Carbon Nanotubes in Strong Acids
• From Bucky Pearls to Armchair Quantum Wires

**(22b) Nanostructured Scaffolds for Tissue Engineering**
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Helical Rosette Nanotubes as a Biomimetic Tissue Engineering Scaffold Material
• Inverted Colloidal Crystal Hydrogel Scaffold Modified with Layer-by-Layer Assembled Single-Wall Carbon Nanotubes as a Model System for Three-Dimensional Neuronal Cultures
• Electrospun Biomimetic Materials for Cell Targeting Applications
• Fabrication of Novel Tissue Engineering Scaffold Using Nanofibrous Polyaniline and Nonwoven Poly(Ethylene-Terephthalate) Fibers
• Electrospinning of Novel Tricalcium/Poly(Lactide-Co-Glycolide) Nanocomposites for Repair of Bone Defects
• Developing Biosensors for Monitoring Orthopedic Tissue Growth
• From Nano to Micro: Nanostructured Titania/PLGA Orthopedic Tissue Engineering Scaffolds Assembled by Three-Dimensional Printing

**(22b) Symposium on the 65th Birthday of Prof. Clark Colton Part I**
***Hilton San Francisco, Continental 5***
• Clark Colton and the Massachusetts Institute of Technology Graduate Course "Chemical Engineering in Medicine"
• From Enzymatic Regeneration of Atp to Novel Biomaterials
• Biological Engineering: past, Present and Future Trends
• Biology in Engineering, and NSF
• Exploring Enzymology for New Industrial Syntheses
• Engineering Issues in Cell Based Insulin Replacement Therapies

**Advances and Case Studies in Crystallization and Post Crystallization Processing - II**
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• Modeling and Simulation of Impinging Jet Crystallizers
• Effect of Ostwald Ripening on Particle Breakage in Saturated Solutions
• Monitoring of Crystallization Processes: a Novel Approach for the Separation of Touching Edges in Crystal Particle Images
• Relating Chord-Length and Size Distributions: Applications in the Batch Crystallization of Paracetamol
• Simulation of Anti-Solvent Crystallization by CFD-PBE Approach
• Semibatch Evaporative Crystallization of Multiple Solutes
• Filtration, Washing and Sizing of Multiple-Solute Crystal Products

**Advances in Animal and Plant Cell Culture Process Development**
***Hilton San Francisco, Continental 9***
• Increasing Adeno-Associated Virus Volumetric and Specific Yield in Insect Cell Culture by Increasing Temperature and Cell Density
• Antibody Production in the GS-NS0 System under Normal and Hyperosmotic Culture Conditions: a Combined Modeling and Experimental Study
• Implementation of Online Amino Acid Analysis for Medium and Feed Optimization in Mammalian Cell Culture
• Automated Flow Cytometry for Monitoring and Control of CHO Cell Cultures
• Rapid and Efficient Strain Evaluation Using a Micro-Scale Bioreactor
• The Use of Energy Dissipation Rate as a Parameter to Assist in the Evaluation, Scale-up, and Scale-down of Bioprocesses
• Evaluating Biopharmaceutical Economics and Capacity with Process Modeling and Simulation Tools

**Advances in Biochemical Engineering: Honoring Harvey Blanch I**
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• Transport in Vessel Walls: Why Some Vessels Get Atherosclerosis and Others Don't
• New Bacterial Communication Lines by Directed Evolution of Lux R
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• A New Approach for the Solution of Noisy Black-Box Models Involving Integer Variables
• Improving the Integrality Gap Using a Novel Continuous-Time Scheduling Formulation Applied to a Challenging Industrial Benchmark Problem
• Continuous Time Formulation for the Scheduling Optimization of a Mixed Plant with Fixed Batch Processing Time
• Scheduling Complex Job-Shop with Re-Entrant Flow as Partially Observable Markov Decision Process (POMDP) – Application to Semi-Conductor Manufacturing
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• Evolution of Force Anisotropy in a Tilted Granular Bed
• Dimensionless Spray Flux - Effect of Rewetting
• Effect of Peptizing Agents on Pre-Extruded Pseudoboehmite Powder
• Theoretical and Experimental Study of Wet Granulation in Fluidized Bed: Comparison of Experiments with Models of Different Complexity
• Model Predictive Control of Wet Granulation Using an Experimentally Validated Population Balance Model
• Modeling the Agglomeration Process in Fluidized Bed Granulation: A Simple Approach

### Biological Polymers
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Direct Monitoring of the Conformational Change of Elastin-like Polypeptides upon Changing Ionic Strength Using Dual Polarization Interferometry
• Patchy Interactions of Globular Proteins
• Discrete Binding Ranges of Ligated Biopolymers End-Grafted to an Interface: a Theoretical Study
• Complex Formation between Stereoregular Polyelectrolyte and Protein
• Wrapping Transitions in a Single Nucleosome under Tension
• Poly(Glu) and Poly(Glu:Ala) Fibril Formation and $CaCO_3$ Templating Ability
• Effects of Fluid Shear on the Conformation of Human Von Willebrand Factor Studied by Neutron and Light Scattering
• Characterization of Swelling Behavior of Cross Linked Waxy Maize Starch Dispersions

### BioMEMS and Microfluidics: Biomedical Diagnostics
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• A Fully Automated Nanoliter Viscometer for Analyzing Newtonian and Non-Newtonian Body Fluids and Polymeric Liquids
• A Novel Application of Isotachophoresis to Enhance Immunodiagnostic Assays on a Microchip
• Purification of Genomic DNA from Whole Cell Lysates Using Photoactivated Polycarbonate Microfluidic Devices
• Delivery of Molecules and DNA into Mammalian Cells by Electroporation on a Microfluidic Device
• On-Chip Electrochemistry Based Real Time Polymerase Chain Reaction

### Biomolecules at Interfaces I - Protein-Membrane Interactions and Proteins at the Air-Water Interface
***Hilton San Francisco, Union Square 22***
• Molecular Dynamics Simulations of Lipid-Protein Interactions
• Interfacial Properties of Alzheimer Amyloid- ß Peptides in Various Self-Assembled Forms
• An Investigation of the Functionality of Synthetic Peptides in Pulmonary Surfactant Formulations from Molecular Dynamics Simulations
• Cell Membrane Ganglioside $G_{M1}$ Mediated Amyloid-Beta Fibril Formation and Membrane Disruption
• Ampetoids: Functional Mimics of Helical, Cationic Antimicrobial Peptides
• Cholera Toxin Assault on Lipid Membranes Containing Ganglioside Gm1: an X-Ray Reflectivity and Grazing Incidence Diffraction Study at the Air-Water Interface
• Understanding Competitive Adsorption at the Air-Water Interface to Reverse Surfactant Inactivation in Acute Respiratory Distress Syndrome
• Adsorption Dynamics of Components of Pulmonary Surfactant at the Air/Water Interface
• Characterization of Self-Assembled Protein Films at the Air-Water Interface Using the Cambridge Interfacial Tensiometer
• Prueba De Articulo

### Colloidal & Interfacial Phenomena in Aquatic Systems
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• Colloids, Contaminants, and Surface Chemistry: Effect of Desorption Kinetics on the Facilitated Transport of Cesium and Strontium by Illite Colloids
• Clogging by Montmorillonite in Porous Media: Hydrodynamic and Chemical Effects
• Particle Deposition Onto Chemically and Topologically Heterogeneous Surfaces
• *E. Coli* Deposition and Transport in Porous Media: Influence of Solution Chemistry and Bacterial Surface Polymers
• Adhesion of Plasmid DNA to Natural Organic Matter Coated Mineral Surfaces
• Diffusivity Measurements of Bacteriophages by Gradient Diffusion and Dynamic Light Scattering
• Biofouling of Organic and Chemically Modified RO/Nf Membranes

### Critical Issues in Information Technology
***Hilton San Francisco, Continental 3***
• Marshalling the Cyber Infrastructure to Solve Big Problems
• Better Plant Startup Via Simulation
• Smart Plants: a New Opportunity for Industry and University
• The Smart Plant - Fully Realizing the Opportunities for Industry
• Roundtable on Critical Issues in Information Technology

### Curriculum Revision
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• Transforming the Educational Experience of Transfer Students in Chemical Engineering Using a Multi-Dimensional Spiral Curriculum
• A Flexible Chemical Engineering Curriculum
• Curricular Reform at Tennessee Technological University
• "Tracks" for Specialization within a ChE Education
• Curriculum Revisions for the (Bio)Chemical Engineer

### Developments in Thermochemical and Electrolytic Routes to Hydrogen Production: Part I
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• Experimental Results for the Generation of Hydrogen by the Decomposition of Hydrogen Iodide in the Sulfur-Iodine Cycle
• Hi Concentration by Electro-Electrodialysis from HIX Solution (Hi-I2-$H_2O$ Mixture) for Hi Decomposition Reaction in Is (Iodine-Sulfur) Process
• Advances in Acid Concentration Membrane Technology for the Sulfur-Iodine Thermochemical Cycle
• Inorganic Membranes to Facilitate the Production of Hydrogen Using Nuclear Energy
• Process Flowsheet Analysis of Hydrogen Iodide Decomposition in the Sulfur-Iodine Cycle

### Dynamics and Modeling of Particles, Crystals and Agglomerate Formation
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• Kinetics and Modeling of Crystallization in Surfactant-Free Monodisperse Emulsions
• The Influence of Nucleation Kinetics on the Particle Population Dynamics in Microemulsion Precipitation Using Molecular Modeling Approaches
• Numerical Simulation of $BaSO_4$ Precipitation in a Coaxial Pipe Mixer with Micromixing Effects
• Non-Isothermal Crystallization Kinetics of Waxy Crude Oils
• Aggregation with Collision-Induced Breakage: Solutions and Comparison with Linear Breakage
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• Adsorption of Low Molecular Weight Perfluoroalkanes on Nanoporous Carbon
• Structure Promoted Ca-Based Sorbents for Highly Reversible Carbon Dioxide Uptake at High Temperatures
• Molecular Modeling of Carbon Dioxide Adsorption on Coal-like Adsorbents
• Experimental and Modeling Study of the Adsorption of $CO_2$ on Coal Aimed at Ecbm Recovery
• Adsorption of Carbon Dioxide on Alkali Metal Exchanged Zeolites

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• Molecular Dynamics Simulation of Simple Gases in Various Porous Structure Models
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**Identification and Application of New Solvents and Processes for Separations**
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• Using Tunable Solvents to Couple Biphasic Extraction with Homogeneous Reactions
• Visualization of Mass Transfer from an Electrically Charged Pendant Drop
• Chemical Reaction with Extraction - Investigation of Catalysts for Synthesis of Methyl Acetate
• Nonisothermal Dynamic Model of a Supercritical Fluid Extraction Packed Column
• Optimization of Whole Broth Extraction: a Case Study of Secondary Metabolite Isolation

**Incorporating New Technologies into Chemical Engineering Education**
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• Synergism of Multi-Disciplined Coordination in Undergraduate Heat Transfer Education
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• Molecularium: Merging Entertainment with Education, Outreach, and Scientific Literacy
• Nanotechnology in Undergraduate Engineering and Science Education
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• Young Engineers & Scientists Seminars: a High School Enrichment Program
• Introductory Biomedical/Biochemical Engineering Elective

**Interfacial Phenomena in Environmental Systems**
***Hilton San Francisco, Union Square 21***
• Force Measurements between Cryptosporidium Parvum Oocysts and Positively and Negatively Charged Colloidal Particles
• Foam for Mobility Control in Enhanced Oil Recovery Processes Using Surfactants
• Super-Hydrophobic Porous Silicon Surfaces
• Toner Particle - Bubble Interactions in Deinking Flotation
• Hydrolytic Degradation of Polylactide and Production of Water-Soluble Hydrolyzate Species
• Effect of Polymer and Protein Surface Coatings on Silicone on Staphylococcus Epidermidis Adhesion and Colonization
• Effect of Inorganic Solids, Wax to Asphaltene Ratio, and Water Cut on the Stability of Oilfield Emulsions

**Invited: Alpha Chi Sigma Symposium**
***Hilton San Francisco, Plaza A***
• Self-Organized Large Area Patterning of Soft Solids by Elastic Contact Lithography
• Granular Matter: Origins, Linkages, and Recent Vignettes
• Spatial and Temporal Control over the Self-Assembly of Surfactants
• An Elementary Kinematical Model of Thermal Diffusion in Liquids and Gases
• Inhaling Cationic Aerosols to Mitigate the Spread of Infectious Disease
• Physical and Chemical Characterization of Foods
• Fluid Film: a Tool for 2d Nano-Matter Self-Assembly

**Invited: In Honor of Neal Amundson's 90th Birthday, I**
***Hilton San Francisco, Imperial A***
• Vision Accomplished: Computer-Enabled Functional Analysis of Coating Flows
• "Wall Enhanced Dispersion in Cylindrical Packed Beds"
• Block Copolymer Surfactants
• Hydrogen and Chemicals in Millisecond Reactors
• Rational Design of Shape Selective Molecular Sieves
• Stability and Instability in Complex Isothermal Chemistry: the Big Picture

**Invited: Thermodynamic Properties and Phase Behavior I: Honoring the Contributions of John M. Prausnitz**
***Hilton San Francisco, Continental 6***
• Solubility of Sour Gases in Aqueous Solutions of Amines
• Practical and Rational Design of Bioseparation Processes Using Correlative Thermodynamic Models
• Phase-Equilibria in Polymer Systems – Experiments and Modeling
• Surfactant Adsorption Thermodynamics at Fluid/Fluid Interfaces Studied with Diblock Copolymers
• Participation of Molecular Simulation in the Development of Molecular-Thermodynamic Models
• Drug Design, Development and Delivery: Integrated, Interdisciplinary Education in Pharmaceutical Science

**Manipulation of Nanophases by External Fields**
***Hilton San Francisco, California Room***
• Surfactant-Coated Nanoparticle on a Stepped Surface
• Observation of the Nucleation and Growth of CdS Nanocrystals in a Two-Phase System
• Simulation of the Hydrodynamically-Assisted Self-Assembly of DNA-Functionalized Colloidal Particles in 2d
• Controlled Deposition of Nanoparticles on a Solid Substrate: Numerical and Experimental Investigation of the Effect of Fluid Flow Both in the Absence and Presence of External Electric Field
• Recent Advances in Nanoscale Thermal Lithography Using Heated Atomic Force Microscope Cantilevers and Cantilever Arrays
• The Role of Magnetic and Electric Fields in Membrane-Based Separation of Aqueous Electrolyte Solutions
• Preparation of Calcium Alginate Microbeads by Electrodispersion for Protein Drug Controlled Release

**Materials Synthesis and Processing with near and Supercritical Fluids II**
***Hilton San Francisco, Union Square 3 & 4***
• Supercritical Carbon Dioxide Dispersion of Nano-Clays and Clay-Polymer Nanocomposites
• Synthesis and Steric Stabilization of Silver Nanoparticles in Neat Carbon Dioxide Solvent Using Fluorine-Free Compounds
• Application of Sfe Extraction in a Countercurrent Column with Structured Packing for Recovery of Purified Squalene from Oil Residues
• Rotational Rheometry of Polystyrene under High-Pressure Carbon Dioxide
• In-Situ Fluorescence Spectroscopy Investigation of Supercritical Carbon Dioxide Swelling of Surfactant Templates in Porous Silica Thin Films
• Solvation Effects in Low Temperature Supercritical $CO_2$-Based Heterogeneous Thin Film Deposition Reactions
• Synthesis of Titanium Dioxide Photocatalyst with Tunable Nanoporosity Using of Supercritical Fluids

**Membrane Session Honoring Professor Ed Ma - II**
***Hilton San Francisco, Yosemite C***
• High Aspect Ratio Mixed Matrix Membranes: Advantages and Challenges
• Preparation of Hydrogen-Permselective Silica Membranes Having a Bimodal Catalytic Structure and Application to the Steam Reforming of Methane
• Corrosion-Resistant Zeolite Coatings for Metals and Alloys
• From Zeolite Nanocrystals to Zeolite Films and Membrane
• Zeolite Thin Film-Fiber Integrated Microsensors for Studying Molecular Transport in Zeolite Membranes
• Energy Related Zeolite Membrane

**Membrane Tutorial II**
***Hilton San Francisco, Yosemite B***
• Polymeric Membranes for Molecularly Selective Hydrocarbon Separations
• Microporous and Dense Inorganic Membranes
• Ultrasonic Reflectometry for Membrane Applications: Current Work and Future Opportunities

**Mixing in Microdevices and Microreactors I**
***Hilton San Francisco, Union Square 19 & 20***
• On-Chip Dispersion Measurement in Segmented Flow through Microchannels
• Dispersion Effects of Microchannel Configurations and Turn Geometries
• Fractal Patterning for Mixing Enhancement in Microchannels
• Elimination of the Isolated/ Stable Region in 3d Chaotic Micromixer through Reorientation Process
• Rates of Diffusion-Limited Reactions in Stirred Microfluidic Flows
• Mixing Size Control and Mass Transfer Performance in a Microfluidic Device

**Multiphase Polymers in Honor of Stuart L. Cooper's 65th Birthday**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Specialty Applications of Ionomers
• Functional Thin Film Coatings Based on Ion-Containing Block Copolymers
• Creating Functional Polymer Surfaces with Block Copolymers
• Segmented Polyurethane from Soyoil Polyols
• Hydrophobic - Polyelectrolyte Block Copolymers for Surface Modification

**Multiscale Modeling of Nanoparticle Systems**
***Hilton San Francisco, Franciscan C***
• Study of Water Adsorption on Nanoparticle Surface and Phase Transformation during Nanoparticle Sintering Via Molecular Dynamics Simulations of Tio2 Nanoparticles
• Molecular Dynamics Simulation of Nanoparticle Self-Assembly at a Liquid-Liquid Interface
• Molecular Dynamics Simulation of Nano-Scale Lubricant Films in Humidity
• Molecular Dynamics Modeling of Nanodroplet Spraying on Liquid Substrates
• Collection Efficiency of Nanosize Particles in an Electrostatic Precipitator
• Modeling Aqueous Environments in Pre-Nucleation Silicate Species
• Slip Flow in Nanofluidics: Slip Length Vs. Contact Angle on Hydrophobic Surfaces from Nonequilibrium Molecular Dynamics

**Nanoparticle Manipulation and Separation**
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Synthesizing Complex Nano-Colloid and Nano-Fiber Morphologies by DC and AC Electrosprays
• Filtration of Submicron Particles by Agglomerates of Nanoparticles

• Effect of Electric Field on the Hydrodynamics of Nanoparticles in a Rectangular Fluidized Bed
• Forced Assembly of Cobalt Nanoparticles
• Manipulation and Control of the Particle Size Distribution of Nanoparticles during Their Formation in Microemulsion Droplets by a Suitable Feed Strategy
• Separation of Polydisperse Metal and Semiconductor Nanoparticle Populations into Monodisperse Fractions Using $Co_2$ Expanded Liquids

**National Student Design Competition**
***Hilton San Francisco, Taylor***

**Particulate and Multiphase Flow**
***Hilton San Francisco, Union Square 15 & 16***
• The Dynamics of Rodlike Particles under Sedimentation and Induced-Charge Electrophoresis
• Multiphase Modeling of Electro- and Magnetorheological Suspensions
• A Continuum Framework for the Description of Mixing and Segregation in Three-Dimensional Granular Flows
• Wall-Induced Particle Migration and Ordering Mechanisms in Dilute Suspensions of Spherical Particles in Creeping Flow Conditions
• The Effect of Second Normal Stress Difference Induced Secondary Currents on the Concentration and Velocity Distributions for Suspension Flow in Different Geometries
• Shear Induced Particle Migration in Binary Colloidal Suspensions
• Pressure Drop and Flow Evolution of a Concentrated Suspension in an Abrupt Expansion
• Competition between Particle Migration and Chaotic Advection in Microchannels
• Squeezing of Deformable Drops through Granular Materials
• Dynamic Simulations of Soft Particle Pastes

**Plenary Session II: US-Japan Joint Topical Conference on Medical Engineering, Drug Delivery Systems and Therapeutic Systems**
***Hilton San Francisco, Continental 4***
• Terminus-Dependent Phenomenon of DNA-Functionalized Nanoparticles for Microchip DNA Sensing
• Smart Drug Delivery Systems That Learn from Nature
• Sixty Years of Artificial Organs Development — from Rotating Drums to Nanotechnology

**Plenary Session on Opportunities and Challenges in Product Design**
***Hilton San Francisco, Grand Ballroom A***
• Designing Chemical Products
• Product Development: from Conceptualization to Market
• Creating and Implementing Medical Technology
• Panel Discussion

**Process Monitoring and Fault Detection I**
***Hilton San Francisco, Union Square 5 & 6***
• Diagnosis of Oscillating Control Loops
• Integration of Data Rectification and Incipient Process Fault Diagnosis
• Process Trend Monitoring Based on Key Sensitive Index: Applications Semiconductor Manufacturing
• Statistical Fault Detection of Batch Processes in Semiconductor Manufacturing
• Real-Time Thin Film Characterization during Chemical Vapor Deposition Using Moving Horizon Estimation
• Industrial Implementation of on-Line Multivariate Quality Control (Part II: Long-Term Performance, Model Maintenance, and Model Leveraging)
• Evolving Models and a PLS Similarity Factor for Monitoring Batch Processes
• Bio-Reactor Monitoring with Multiway-Pca and Model Based-Pca
• Variance Component Analysis Based Fault Diagnosis of Multi-Layer Overlay Lithography Processes

**Processing of Pharmaceuticals and Neutraceuticals under High Pressure**
***Hilton San Francisco, Union Square 1 & 2***
• Micronization of Pharmaceutical Powders by High Pressure Homogenization in Compressed Fluid Antisolvents
• Mechanisms of Supercritical Carbon Dioxide Sterilization of Bacterial Spores
• Inactivation of Microorganisms by High Pressure Carbon Dioxide Treatment
• Extraction of Complex Lipids from Aqueous Streams Using near-Critical Dimethylether
• Biocompatible Polymers Characterization by inverse gas chromatography

**Properties and Characterization of Nanocomposites**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Ubiquity of Soft Glassy Dynamics in Polypropylene-Clay Nanocomposites
• Quiescent and Flow-Induced Crystallization of Polypropylene-Clay Nanocomposites
• Molecular Dynamics Simulation of Na-Montmorillonite Nanocomposite Materials
• Strain Hardening in Elongational Flow of Nylon-Clay Nanocomposite Melts
• MWNT-Percolated Epoxy Network Composites: Synthesis and Characterization
• Anisotropy in Layered Polymer-Clay Nanocomposites
• Polymeric Nanofoams for Industrial Applications

**Stability and Nonlinear Hydrodynamics**
***Hilton San Francisco, Union Square 17 & 18***
• The Axisymmetric Instabilities of Electrically-Driven Viscoelastic Jets
• Response of Liquid Jets to Internal Modulated Ultrasonic Radiation Pressure
• Stability of the Shape of a Cusped Bubble Rising in a Viscoelastic Fluid
• Spatio-Temporal Pattern Formation in Viscoelastic Taylor-Couette Flow: Dynamical Simulation and Mechanism
• Effect of Radius Ratio on Flow Transitions in Newtonian Taylor-Couette Flows
• Effect of Prandtl Number on the Dynamics and Stability of Natural Convective Flows inside a Cubical Cavity
• A Free-Boundary Theory for the Shape of the Ideal Dripping Icicle
• Finite-Amplitude Deformation of Liquid Films Subjected to Electric Fields
• Flow Reversal and Eddy Formation in Thin Film Flows
• Large-Scale Bifurcation and Stability Analysis of Cfd Applications

**Student Poster Session: Catalysis & Reaction Engineering**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Computing & Process Control**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Education**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Environmental**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Food, Pharmaceutical & Biotechnology**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Fuels, Petrochemicals & Energy**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: General Papers**
***Hilton San Francisco, Grand Ballroom B***
• Antimicrobial and Hydrophilic Zeolite Coating
• Electrokinetic-Based Drug Delivery through the Skin
• Impact of Auto-Exhaust on the Environment of Dhaka City

**Student Poster Session: Materials Engineering & Sciences**
***Hilton San Francisco, Grand Ballroom B***

**Student Poster Session: Separations**
***Hilton San Francisco, Grand Ballroom B***

**Supercritical Fluids for Food and Pharmaceuticals**
***Hilton San Francisco, Union Square 25***
• Improving Physical Characteristics of Insulin Powder for Pulmonary Delivery by Addition of Stabilizers
• Fluid-Filled Microcapsules for the Food Industry
• Supercritical Precipitation of Acyclovir
• Gentle Drying of Sensitive Food Products
• Influence of Operating Variables on Particle Size and Morphology in High Pressure Carbon Dioxide Antisolvent Process
• Compressed Fluid Based Process for Development of Cosmetic Products
• Numerical Study of the Effect of Fluid Dynamics on Particle Formation in a Conventional SEDs Apparatus

**Systems Analysis of Sustainability**
***Hilton San Francisco, Continental 7***
• Chemical Process Assessment and Design Based on Green Degree Method
• Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives
• Exergy Recuperation Technology for Energy and Materials Co-Production
• Fisher Information as a Metric for Sustainability
• Sustainable Production of Gasohol from Biomass
• Agent-Based Modeling and Simulation to Complex Adaptive Eco-Industrial Systems
• Optimal Control Theory for Sustainable Environmental Management

**Tissue Engineering: Biomaterial-Cell Interactions in Tissue Engineering (II)**
***Hilton San Francisco, Continental 8***
• Nanoscale RGD Peptide Organization and Substrate Elastic Modulus Regulates Stem Cell and Pre-osteoblast Proliferation
• Cell-Matrix Interactions: Quantifying Cell Migratory and Contractile Behavior in a Series of Characterized Collagen-Gag Scaffolds
• Engineering the Alginate Matrix Regulates Tissue Development and Growth of Ovarian Follicles
• Extracellular Matrix Chemistry and Mechanics Cooperatively Regulate Smooth Muscle Cells
• Effects of Long Term Cyclic Strain on Fibrin Based Cylindrical Tissue Constructs
• Eliminating Oxygen Supply Limitations for Transplanted Microencapsulated Islets in the Treatment of Type I Diabetes
• Monitoring Dissolved Oxygen Concentrations in Tissue Engineered Substitutes

**Transport at Interfaces I**
***Hilton San Francisco, Union Square 23***
• Mass Transfer from Growing and Oscillating Rising Bubbles
• Effect of Viscous Forces on the Measurement of Surface Dilatational Moduli with Oscillating Drops or Bubbles
• Nonlinear Dynamics of Breakup of Surfactant-Laden Compound Jets
• Surfactant-Enhanced Thermocapillary Flows
• Study of Mass Transfer across Liquid-Liquid Interphase Using Micro Visualization Technique
• Adsorption Dynamics of Aqueous 1-Octanol Solutions at the Vapor / Liquid Interface
• Transport Coefficients for Liquid-Vapor Transition

**Transport Processes in Multiphase Systems II**
***Hilton San Francisco, Union Square 14***
• Keynote Lecture: Gas Transfer and Turbulence at the Air-Water Interface
• Mass Transfer across the Air-Water Interface
• Gas Transfer and Surface Divergence at a Wind Sheared Air-Water Interface
• Performance Enhancement in a Direct Methanol Fuel Cell Via an Externally Applied Oscillatory Flow
• A Fuel Cell Motivated Model for the Decay of Bubbles Due to Coalescence in Small Channels
• Interfacial Area in a Packed-Bed Reactor Operating in Trickle Flow Regime
• Transport of Liquid Water under Tension in a Synthetic Tree
• Momentum Stress Jump Condition at the Fluid-Porous Boundary: Prediction of the Jump Coefficient

**MONDAY, 13 NOVEMBER 2006**
***3:15 PM - 5:45 PM***
**(22a) Issues in Carbon Nanotubes III: Adsorption and Transport**
***Hilton San Francisco, Franciscan D***
• Fast Mass Transport through Sub-2nm Carbon Nanotubes
• Nano-Scale Transport Phenomena in the Ionic, Solvent and Gaseous Regimes through Carbon Nanotube Membranes
• Experimental Measurement of Pure-Gas Diffusivities in Carbon Nanotubes by ZLC Technique
• On the Mechanism of Water Diffusion in Narrow Carbon Nanotubes
• Diffusion Studies of Water and n-Alkane Molecules in Carbon Nanotubes
• Neon Adsorption Isotherm Studies on Single Walled Carbon Nanohorns

**(22b) Nanostructured Biomimetic and Biohybrid Materials and Devices**
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Autonomous Molecular Muscle with a Brake
• Design and Computational Analysis of Protein Based Nanoscale Biomimetic Actuators
• Molecular Recognition Ion Gating Membrane and Its Nonlinear Oscillation Response
• Biomimetic Interfaces Based on Membrane Proteins for Bioelectronic Applications
• Nanostructured Self-Assembled Reversible and Directional Bio-Molecular Templates for Nanotechnology Interconnects
• Efficient Enzymatic Manipulation of Nanoparticle-Bound DNA to Form Nanoparticle-DNA Conjugates Bearing Specific Number of Short DNA Strands
• Bioinspired Vesicle Restraint and Mobilization Using a Biopolymer Network
• 3d Nanostructured Microenvironments for *in-Vitro* Hematopoietic Stem Cells Niches
• Fabrication of Nanopatterned Dots of Proteins by Particle Lithography

**(22b) Polymers as Functional Components of Micro- and Nanodevices**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Design of a Novel Injectable Polymer Scaffold for Spinal Cord Repair
• Glucose-Responsive Systems for Insulin Delivery Based on Poly(Ethylene Glycol)-Containing, pH-Sensitive, Cationic Hydrogels
• Novel Valving and Packaging Designs for Protein Containing Biochips
• Tunable Biomolecular Recognition Films for Sensing
• Intelligent Hydrogel Systems as Functional Coatings on Magnetic Nanoparticles
• Characterization of Actin-Based Motility on Patterned Substrata
• Cylindrical Micro-Porous Membranes for Directed Cellular Growth
• Development of Quantum Dot Encoded Polystyrene Beads for Use in an Ultra-Miniaturized Microarray Platform
• Coupled Translational and Rotational Fluctuations of Tethered Beads
• Development of Poly(Ethylenimine) Based Redox Polymers for Biosensor Devices

**(22b) Symposium on the 65th Birthday of Prof. Clark Colton Part II**
***Hilton San Francisco, Continental 5***
• Diffusive Movement of Molecules and Cells in Flowing Blood
• The Evolution of Hemodialysis since Clark Colton's Doctoral Thesis
• Real-Time Sampling, Concentrating and Measuring of Airborne Aerosols
• Reaction-Enhanced Acid Gas Transport in Membranes and Absorbers
• Protein Transport in Nanoporous Membranes
• Chromatographic Refolding of Proteins

**Advances in Biochemical Engineering: Honoring Harvey Blanch II**
***Hilton San Francisco, Plaza B***
• Bioprocess-on-a-Chip
• A Gene-Ontology Driven Analysis of Complex Phenotypes
• Nicotinamide (Vitamin B3) Increases the Ploidy and Proplatelet Production of Human Megakaryocytes
• Microscale Tissue Engineering for Drug Discovery and Development
• Ustar - the Universal Sequence-Tag Array Technology for Absolute Quantification of Per Cell Transcript Profiles
• Engineered Strategies to Overcome Multidrug Resistance in Solid Tumors
• Understanding the Role of Culture Conditions on Specific Productivity in Cultured Mammalian Cells

**Advances in Protein Expression and Post-Translational Modification**
***Hilton San Francisco, Continental 8***
• Exceptional Total and Functional Yields of the Human Adenosine $a_{2a}$ Receptor Expressed in the Yeast *Saccharomyces Cerevisiae*

• Enabling Biosynthesis of Complex Proteins in Bacteria Via Ribosome Reprogramming
• Humanization and Structural Studies to Tailor the Efficiency of Pertussis Toxin (Pt) Neutralizing Antibodies
• Cellular and Protein Engineering Approaches for Increasing Human Brain-Derived Neurotrophic Factor Production in Yeast
• Engineering Membrane Protein Biogenesis
• Directed Evolution of a G-Protein Coupled Receptor
• Cell-Free Protein Synthesis of Complex Proteins Containing Unnatural Amino Acids

### Agglomeration and Granulation Processes II
***Hilton San Francisco, Franciscan B***
• Binder Selection in Pharmaceutical Granulation: Wetting, Spreading, Stickiness and Strength
• Granulation of Hydrophobic Powders Via Solid Spreading Nucleation
• The Microscopic Study of Granulation Mechanisms and Their Effect on the Non-Uniformity of Granule Properties
• Top-Spray Fluidized Bed Coating: Scale-up Using Response Surface Methodology
• Study of the Mechanisms during Drying of a Pharmaceutical Fluid Bed Granulation: Correlation of Residual Water Content with the Chemical Stability of the Formulation
• Modeling of Growth Kinetics of Wet Granulation in a High Shear Mixer by Means of Image Processing and Analysis

### Applications of Adsorption in Reactive and Non Reactive Processes
***Hilton San Francisco, Sutter***
• Effects of the Solvent on Catalytic Isomerization of 1,5-Dimethylnaphthalene and Adsorption of 2,6-Dimethylnaphthalene
• Overcoming Product Inhibition by Adsorptive Reactor
• Non-Equilibrium Kinetic Model for the Reversible Adsorption of Carbon Dioxide on a K-Promoted HTLC
• Modeling of Industrial PSA Process for Fuel Ethanol Production
• A Four-Bed PSA for Clean Separation of Ethylene-Ethane Mixture
• Ion-Exchange Equilibrium and Fixed-Bed Performance of the System Vanillin/NaOH-Amberlite Ir 120h
• Adsorption Isosters Measurements on CaCl2 Impregnated ACF Felt for an Application of Ammonia Scrubber

### Applications of Fluidization
***Marriott San Francisco, Yerba Buena Ballroom 6***
• The Effect of Gas and Particle Properties on the Fluidization State of APF and ABF Nanopowders
• Fundamental Bubbling Characteristics in a Rotating Fluidized Bed
• Prediction of Propensity to Fouling in Fluid Cokers
• Development of a Multi-Scale, Multi-Phase, Multi-Zone Dynamic Model for the Prediction of Particle Segregation in Catalytic Olefin Polymerization FBRS
• Application of a Fluid-Particle Mass Transfer Model for the Sorbent Injection Process for Mercury Emission Control during Coal Combustion
• Further Investigation into Regime Transition from Bubbling to Turbulent Fluidization
• Wide Spanned Minimum Spouting Velocity Correlations Based on a New Quantitative Measurement and Identification Procedure

### B.S. Ch E: What Is It?
***Hilton San Francisco, Van Ness***
• Trends in Engineering Educational Research and Curriculum Reform
• Tuning the Chemical Engineering Curriculum to Meet New Challenges and the Demand of the Job Market
• Looking out a Few Years
• Semiconductor Education in the Chemical Engineering Curriculum
• ChE – the Most Versatile Degree
• Chemical Engineering - the Liberal Arts Degree for the Next Century

### BioMEMS and Microfluidics: Sensing, Detection, and Integration
***Hilton San Francisco, Yosemite A***
• Rapid Pathogen Detection with Integrated AC Electrokinetic Devices
• Microstencils for Patterning of Nontraditional Materials
• Comparison of Microfluidic Protein Patterning Methods Onto Waveguide Surfaces
• Study of FET Flow Control and Electrostatic Response of Charged Molecules in Nanofluidic Channels
• Spatially Controlled Chemistry Using Remotely Guided Nanoliter Scale Chemical Containers
• Nanostructure Based Biomimetic Interfaces for Bioelectronic Applications

### Biomolecules at Interfaces II - Sensing and Exploiting Heterogeneities
***Hilton San Francisco, Union Square 22***
• Detection and Characterization of Lipid Rafts by Fluorescence Spectroscopy
• Effect of Transmembrane Distribution of Fluid-Gel Patterned Bilayers
• Diffusing Colloidal Probe Measurements of Protein and Synthetic Macromolecule Interactions
• Fractal Analysis of Interleukin Binding and Dissociation Kinetics on Biosensor Surfaces
• Study of Enzyme-Lipid Membrane Interaction on Model Lipid Membrane Arrays
• Creating Well-Defined, Tailorable Polymer-Tethered Lipid Bilayers
• The Electrical Response of DNA Brushes
• Adsorption of Hydrophobically Modified DNA to Micelles, Liposomes, and Microemulsions
• Mobility of Strongly Adsorbed Biopolymers on Supported Lipid Bilayers

### Co2 Separation, Capture for Sequestration, and Utilization for Sustainable Development
***Hilton San Francisco, Continental 7***
• Pilot Plant Studies and Modeling of $CO_2$ Capture Using an Amp Solution
• Doped Oxygen Carriers for Inherent $CO_2$ Capture Using Chemical Looping Combustion
• Development of a New Recycling Process of Shell Waste Using High-Pressure Carbon Dioxide Solution
• Novel Heavy Reflux PSA Cycles for the Recovery of Carbon Dioxide at High Temperature with K-Promoted HTLC
• Energy Dissipation for $CO_2$ Injection with a Static Mixer for Ocean Sequestration
• Ionic Liquids as Absorption Media for $CO_2$ Capture
• Enabling Sustainable Fossil Fuel Energy Conversion Systems: $CO_2$ and $SO_2$ Mineral Sequestration and Utilization of Solid Byproducts
• Novel High Temperature $CO_2$ Acceptor Using Zirconium-Based Alkali Mixed Oxides
• Development of $CO_2$ Injection Method "Cosmos" for $CO_2$ Ocean Storage

### Colloidal Hydrodynamics
***Hilton San Francisco, Union Square 15 & 16***
• On the Motion of Two Particles Translating with Equal Velocities through a Colloidal Dispersion
• Active and Nonlinear Microrheology in the Large-Probe Limit: Direct Vs. Bulk Effects
• Microstructure Response in a Colloidal Gel Using Laser Tweezers
• Simulations of Particle Transport through Colloidal Gels
• One-Dimensional Diffusion of Colloids in Colloid-Polymer Mixtures
• Noncontinuum Effects in Nanoparticle Dynamics in Polymers
• Particle Phase Pressure in Sheared Suspensions
• Rheology and Structure Formation in Sheared Suspensions of Elastic Particles
• Lift Force on an Asymmetrically Rotating Particle in Confinement
• Catalytic Nanomotor Modeling

### Computational Genomics
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Global Pairwise Sequence Alignment Using Integer Linear Optimization: a Path Selection Approach
• Degenerative Sequence Motifs Identification
• Using Multicellular Pathway Modeling to Gauge the Stability of Tissue Differentiation
• Selection of Informative Genes in Time-Course Gene Expression Data
• A Hierarchical Approach to Identify Phenotype Relevant Pathways
• Metabolic and Genomic Analysis of Acetaminophen Metabolism

### Data Analysis for Process Operations
***Hilton San Francisco, Continental 1***
• Modeling and Optimization of Batch Process Operation through Wavelet Analysis and Multivariate Analysis
• Quality-Based Retrimming Optimization
• Stochastic-Based Accuracy of Data Reconciliation Estimators for Linear Systems
• Integrated Operation Support System (IOPSS): the Data Pre-Processing and Data Reconciliation Modules
• Uniting Data - and Model-Based Fault-Detection Filters for Fault-Tolerant Control of Process Systems
• Comparison of Decision Fusion Strategies for Combining Heterogeneous Diagnostic Fault Classifiers

### Developments in Thermochemical and Electrolytic Routes to Hydrogen Production: Part II
***Hilton San Francisco, Union Square 13***
• Hybrid Sulfur Cycle Flowsheets for Hydrogen Production from Nuclear Energy
• Thermodynamic Modeling for the Hybrid Sulfur Process in ChemCad
• Generation of Hydrogen Using Electrolyzer with Sulfur Dioxide Depolarized Anode
• Electrochemical Generation of Hydrogen Via Thermochemical Cycles
• Investigation of the Reactive Distillation Separation for Hi-$I_2$-$H_2$ in the S-I Process for Thermochemical Hydrogen Production

### Dynamic Simulation & Optimization
***Hilton San Francisco, Continental 2***
• A Comprehensive Framework for Estimation and Dynamic Optimization of Chemical Reaction Systems
• Optimal Operation of a Middle-Vessel Batch Reactive Distillation Process
• Dynamic Re-Optimization and Control under Partial Plant Shutdown Scenarios
• Dynamic Optimization Based on Adjoint Sensitivity Computation
• The Choice of Sensitivity Metrics in Model-Based Design of Optimal Experiments

### Engineering Fundamentals of Drug Delivery
***Hilton San Francisco, Continental 4***
• Improving the Oral Delivery of Macromolecules through the Study of Permeation Enhancers
• Effect of Molecular Weight of Penetrants on Iontophoretic Transdermal Delivery *in Vitro*
• Skin Enzymes Distribution in Transdermal Drug Delivery
• Finite Element Model of Controlled Release Via the Degradation and Erosion of a Polymer Matrix
• Chemotherapy with Drug-Free Hybrid Liposomes
• In Vivo Evaluation of Skin Permeability of Drugs after Applying Adhesive Transdermal Patch
• Physiological Modeling of Gastrointestinal Tract

for Predicting the Effect of Cyclodextrin on Bioavailability of Neutral Compounds

**Entrepreneurial University - Industry Collaborations: Multidisciplinary Structures, Technology Transfer and Women in Technology**
***Hilton San Francisco, Union Square 14***
• Developing Value through Synergistic University/Industry Collaborations
• Can Industry-University Collaborations Converge? a Historical Perspective on Driving Forces
• Industry and Entrepreneurial Partnerships Via Integrated Product and Process Design Courses at the University of Florida
• Small Business Technology Transfer (STTR) Program: Faculty Member Perspective
• Open Innovation, Blurring Organizational Boundaries and the Role of Entrepreneurial University - Industry Relationship
• Careers of Women Scientists and Engineers in Industrial Chemistry: Results from Project Enhance

**Gas Phase Synthesis of Particles**
***Hilton San Francisco, Franciscan C***
• Influence of Gas-Phase Thermodynamics on the Products of Flame Synthesis: from Oxides to Salt and Metal Nanoparticles
• Synthesis of Core-Shell Nanoparticles and Mathematical Modeling of Exponential Relation of Particle Size Variation with Precursor Concentration
• Dual-Plasma Synthesis of Coated Nanoparticles and Nanofluids
• Production of Metallic Bismuth Nanoparticles by Reducing Flame Spray Synthesis
• Continuous Flow Plasma Microreactor Synthesis of Magnetic Nanoparticles
• Mathematical Modeling of Nano-Particle Formation and Evolution in Combustion Processes
• In Situ Observation of Nucleation, Growth and Aggregation in Flame Made Nanoparticles

**Implantable Biomaterials in Honor of Stuart L. Cooper's 65th Birthday**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Welcoming Remarks
• Smart Polymers Then and Now
• Bioactive 3d Gel Matrices in Tissue Engineering
• Engineered Polyurethane Surfaces for Drug Delivery, Blood Compatibility and Tissue Engineering
• Chemical Imaging of Drug/Polymer in Polymer Films by Coherent Anti-Stokes Raman Scattering Microscopy
• Clever Bugs: Microbial Hijacking of the Host Cell Adhesion and Motility Systems

**Incorporation of Product Design into Chemical Engineering Education**
***Hilton San Francisco, Union Square 24***
• Product Design as an Undergraduate Capstone at Columbia University
• Integrating a High-Throughput Screening Lab and Case-Studies into Product Design Courses
• Computer-Aided Product Design
• Capstone Project Design Experiences on Product Design
• Teaching Chemical Product Design
• Management Support for the AIChE National Student Design Competition

**Interfacial Flows I**
***Hilton San Francisco, Union Square 17 & 18***
• Oscillations of Drops Covered with a Monolayer of Insoluble Surfactant
• Surfactant Effects on Drop Detachment
• The Effect of Surfactant and Surfactant Solubility on the Deformation and Breakup of a Bubble in a Viscous Surrounding
• Elastic and Surfactant Effects on Bubbles Rising in a Rectangular Capillary
• Spreading of Surfactant-Bearing Drops on a Solid Surface
• Coalescence of Spreading Droplets on a Wettable Substrate
• Thin Film Drainage and Drop Dynamics in Concentrated Emulsions
• Drop Coalescence in the Presence of an External Flow
• Spontaneous Thermocapillary Interaction of Drops: the Effect of Surface Exothermic Reaction
• Buoyancy-Driven Motion and Deformation of Viscoelastic Drops
• The Effect of Surfactant Solubility on the Deformation and Breakup of a Bubble in a Viscous Surrounding

**Intracellular Processes**
***Hilton San Francisco, Continental 9***
• Inferring Equilibrium Protein Binding Using Fret Imaging Data
• The Effects of PPAR Modulation on Cox-2-Dependent Inflammation and Apoptosis in Shear-Activated Chondrocytes: a Role in Arthritis
• Towards Quantitative Understanding of Mass Transfer in the Endocytic Pathway
• Apoptosis of Human Hepatocellular Carcinoma Cell Is Regulated by Palmitic Acid through the Signal Transduction from PKR to BCL-2
• Involvement of JNK in Cellular Trafficking of Adherents Junction Proteins E-Cadherin and-Catenin: Implication to Cell-Cell Adhesion
• Manipulation and Kinetic Analysis of Crosstalk between Pi 3-Kinase/Ak and RAS/ERK Signal Transduction Pathways
• Analyzing the Stress Response Pathway in *Saccharomyces Cerevisiae*

**Introducing Chemical Engineering to K-12 through Experimentation and Course Integration I**
***Hilton San Francisco, Taylor***
• A Primer for Chemical Engineering Education/K-12
• Project Lead the Way: Introducing High School Students to Engineering

• The Inspires Curriculum: Introducing K-12 Students to Engineering Design Using Inquiry-Based Learning
• Integrating Chemical Engineering as a Vehicle to Enhance Secondary School Science Instruction
• The Great Orange Squeeze: Using Chemical Engineering and the Engineering Design Process to Prepare Middle School Educators for the Massachusetts Engineering Framework Requirements
• Experimental Outreach Activities to Educate High School Students and Attract Them to the Engineering Profession
• Introducing Bioprocess Engineering for K-12 Students
• Using Hands-on Activities to Teach High School Students Chemical Engineering

### Invited: in Honor of Larry Smith, Catalysis and Reaction Engineering Division Practice Award Recipient

***Hilton San Francisco, Franciscan A***

• Some Color Commentary on Innovation
• Experimental and Modeling Studies of Reactive Distillation
• Liquid-Continuous Distillation
• Breaking the Low Temperature Barrier for Sulfuric Acid Catalyzed Gasoline Alkylation

### Invited: In Honor of Neal Amundson's 90th Birthday, II

***Hilton San Francisco, Imperial A***

• AC Field-Driven Dielectrophoresis and Phase Separation in Suspensions
• On Amundson's Legacy
• Thermodynamics of Atmospheric Aerosols
• Optimization Based Predictive Control of Simulated Moving Bed Process Using Subspace Identification
• Solid Acid Catalyzed Alkylation of Isobutane with Butenes
• The Challenges to Our Profession, Especially to Reaction Engineering, in Meeting Future Energy Requirements

### Knowledge Management and Organizational Learning

***Hilton San Francisco, Continental 3***

• Knowledge Management and Organizational Learning? Show Me the Money!
• Embedded Learning Using Wireless Networks and Mobile Computing
• They're Not Just for Compliance Anymore; the Value of Compliance Management Systems in Job-Specific Training
• Instructional Design as a Key Enabler for New Technology Implementation
• Chemical and Reaction Knowledge Discovery for Process Development
• Speeding Innovation through Communities of Practice

### Materials Synthesis and Processing with near and Supercritical Fluids III: Polymers

***Hilton San Francisco, Union Square 3 & 4***

• Fugacity Consideration in Bubble Nucleation of Polymeric Foam Extrusion
• Viscosity and Density of Poly (E-Caprolactone) Solutions in Acetone + Carbon Dioxide Binary Fluid Mixtures
• Solubility and Spinodal Decomposition Analysis for Thermoplastic Foams
• Foaming Using a Polystyrene / Poly(Methyl Methacrylate) Blend and Nanocomposites
• Investigation of Processing and Cellular Structure Formation of Microcellular Polystyrene Foams Using Supercritical Carbon Dioxide
• Solubilities of Blowing Agent Blends
• Nanoparticles Encapsulated in Immobilized Dendrimers: Use of Supercritical Carbon Dioxide as the Processing Medium

### Mathematical Modeling of Transport Processes

***Hilton San Francisco, Union Square 21***

• Off-Lattice Monte Carlo Simulation for Heat Transfer through Carbon Nanotube Composites
• Early Time Analysis of Transport Processes
• Mathematical Modeling of Percutaneous Absorption of Volatile Organic Liquids
• Analytical Modeling of the Forced Gravity Drainage GAGD Process
• Mathematical Modeling of New Phase Growth Due to Solute Diffusion
• Modeling of Non-Newtonian Reactive Systems in Tubular Reactor
• Analytical and Experimental Studies of Mass Transfer and Separation of Species in a Wavy-Walled Tube by Imposed Fluid Oscillation
• Simulations of Miscible Viscous Fingering Phenomena Using Adaptive Discontinuous Galerkin Methods
• Modeling Wave Enhanced Mass Transfer in Falling Films Using Effective Diffusion Coefficients
• Prediction of Tobacco Temperature and Oxygen Profiles in Warehouse Aging Process
• An Analogy between Chemical Reaction and Heat Transfer

### Membrane Reactors

***Hilton San Francisco, Yosemite C***

• Membrane Reactor for the Partial Oxidation of Propylene: Increasing the Yield of Acrolein
• A Hybrid Adsorbent-Membrane Reactor (HAMR) System for Hydrogen Production
• Oxygen Permeable Ceramic Membranes for Hydrocarbon Conversion Reactors
• Diffusion and Release of a Mobile Product in a Reactive Membrane System
• Reductive Degradation of Chlorinated Organics by Membrane-Supported Nanoparticles: Synthesis, Characterization and Modeling Study
• Determining Factors Involved in the Preliminary Design of a Non-Isothermal Membrane Reactor
• Water-Gas-Shift Membrane Reactor for Coal-to-Hydrogen Applications - an Overview
• Hollow Fibre $La_{0.6}Sr_{0.4}CO_{0.2}Fe_{0.8}O_{3-}$ Mixed Conducting Membranes for Oxygen Separation and Methane Combustion

### Microdevices in Separations

***Hilton San Francisco, Mason***

• Microfluidic Device for Nucleic Acid Purification Based on Surface Adsorption to Colloidal Silica
• Miniaturized Hydraulic Pumps with Nanofluidic Structures for Microchip Liquid Chromatographic Devices
• Magnetic Particle Sorting in Microfluidic Devices Fabricated Via Femtosecond Laser Ablation with Surface Modification
• On-Chip High Speed Gas Chromatograph (GC) with Carbon Nanotube Sensors
• Microdevices for the Demonstration of Active Transport through Liquid Crystalline Membranes
• Microfluidic Device for Continuous Particle Separation Using Hydrodynamic Filtration

### Mixing in Microdevices and Microreactors II

***Hilton San Francisco, Union Square 19 & 20***

• Controlling Microfluidic Arrays for Combinatorial Chemistry Using Multi-Functional Valves
• A Microreactor System for Tissue Culture?: Patterns of Colonization and Growth of Mammalian Cells Cultured over Rotating Platforms
• Mixing in the Formulation of Screens for Drug Leads or Crystallization Conditions in Microfluidic Systems
• Gas-Liquid Flow Characteristics in Microreactors
• Modeling of Boiling in Micro-Capillaries by VOF Method

### Novel Techniques for Membrane Characterization and Functionalization

***Hilton San Francisco, Yosemite B***

• Pei/MCM-48 Composite Membranes for Carbon Dioxide Separation
• Modification of Ultrafiltration Membranes by Atom Transfer Radical Polymerization
• Characterization of the Gelation Process in the Preparation of Ppesk Asymmetric Ultrafiltration Membrane
• Surface Modification of Membranes by Initiated Chemical Vapor Deposition
• Characterizing Membrane Surface Charge by Contact Angle Titration
• Surface Energies of Poly(Vinyl Alcohol) Membranes for Pervaporation
• Fundamental Characterization of Surface Mineral Crystallization on Aromatic Polyamide RO Membrane Surfaces
• Surface Modification of Commercial Water Treatment Membranes by Ion Beam Irradiation

### Particle Formation and Crystallization Processes from Liquids or Slurry

***Hilton San Francisco, Lombard***

• Study on Crystallization Phase Diagrams and Kinetics Behaviors of Ketoprofen
• Reactive Crystallization of Pharmaceuticals
• Production of Small API Crystals Via Polymorph Transformation under High Shear
• Real-Time Particle Size and Shape Characterization Using in-Process Video Imaging Process Analytical Technology (Pat) in Dynamic Processes
• On-Line Analysis of Reactive Precipitation Processes
• Scale-up of Anti-Solvent Crystallization Using in Situ Tools and Computational Fluid Dynamics
• Turbidity Spectra and Static Light Scattering in Mie Scattering Regime for Monitoring of Particle Formation Processes

### Process Monitoring and Fault Detection II

***Hilton San Francisco, Union Square 5 & 6***

• Multiblock Process Monitoring and Agent-Based Control of Spatially Distributed Processes
• Optimal Structured Residuals for Multidimensional Fault Isolation Based on Multivariate Principal Component Models
• Analysis of Management Actions, Human Behavior, and Process Reliability in Chemical Plants
• Integrating Fault Diagnosis and Fault-Tolerant Control of Particulate Processes
• Cluster Analysis for Continuous Chemical Process Fault Diagnosis
• Output Feedback Control of Nonlinear Systems Subject to Constraints and Asynchronous Measurements
• A Finite State Machine Framework for Control Performance Monitoring

### Proteomic Systems Biology

***Hilton San Francisco, Union Square 1 & 2***

• A Model for Protein Translation: Polysome Self-Organization Leads to Maximum Protein Synthesis Rates
• Protein Structure and Fold Recognition Using Amino Acid Interaction Models
• Using Atomic Properties to Identify Potential Reactants in Oxidoreductase Reactions
• Initiation of Blood Coagulation: a Systems Biology Approach
• Proteome Changes after Metabolic Engineering to Enhance Aerobic Mineralization of Cis-1,2-Dichloroethylene
• Comparative Metabolic Modeling with Integrated Proteomic Analysis of Synechocystis Sp. Pcc 6803 during Light Versus Dark Cycling
• Integrated Time-Series Metabolomic and Transcriptional Profiling Analyses of *Arabidopsis Thaliana* Response to Elevated $CO_2$ and Osmotic Stress

### Self and Directed Assembly at the Nanoscale

***Hilton San Francisco, California Room***

• Structure and Dynamics of POSS-Based Nanocomposites
• Templated Assembly of Two-Dimensional Hard-Rod Fluids
• Anisotropic Nanoparticles Immersed in Nematic Liquid Crystals

• Computer Simulation of Self-Assembly of Dipolar Colloid Particles for the Design of Stimuli-Responsive Materials
• Self-Assembly of Tethered Nanorod "Shape Amphiphiles" into Novel Staircase and Liquid Crystalline Structures: Insights from Simulation
• Modeling Self-Assembly of Anisotropic Particles for Nanoscale Structures
• Nanowires, Spheroids, Dispersions: the Self-Assembly of Colloidal Nanoparticles

### SMB Separations Technology
***Hilton San Francisco, Powell***
• Continuous Voltage Gradients and Their Application to True Moving Bed Electrophoresis
• Analysis of Zone and Pump Configurations in Simulated Moving Bed Purification of Insulin
• Operation of Simulated Moving Bed in Presence of Adsorbent Ageing
• A Novel Configuration for Gradient Operation in Smb System
• Multicolumn Countercurrent Solvent Gradient Purification
• Full Cycle Optimization of Simulated Moving Bed Processes
• Online Cycle to Cycle Optimizing Control of Varicol and Simulated Moving Bed Processes

### Stimuli Responsive Polymers
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Temperature Responsive and Biodegradable Dendronized Copolymer for Controlled Release of Therapeutic Agents across the Blood Brain Barrier (Bbb)
• Nanoscale Characterization and *in Vitro* Behavior of Poly(Methacrylic Acid-G-Ethylene Glycol) as an Oral Delivery Device for Insulin
• "Smart" Surfaces Formed by Diblock Copolymer Brushes
• Investigation of Tethered Thermoresponsive *n*-Isopropylacrylamide Hydrogel Thin Films Via the Incorporation of Cadmium Selenide/Zinc Selenide Nanoparticles
• pH-Responsive Copolymer Films with Amine Side Chains
• Tethered pH-Responsive Polymer Layers
• Experimental and Theoretical Study of Light-Responsive Poly-Diacetylene Nanocomposites

### Strategies in Biopharmaceutical Scale-up & Pilot Plants
***Hilton San Francisco, Union Square 25***
• Cell Culture Process Scale-up and Technology Transfer for Large-Scale Therapeutic Antibody Manufacturing
• Strategy to Fit a Downstream Purification Platform for an Early Stage Development, Therapeutic Protein into an Existing Pilot Plant
• The Role of Process Modeling in Bioprocess Development and Technology Transfer
• Biologics Pilot Plant Renovation to Enhance Bioreactor and Facility Capacity and Flexibility
• Multi-Dimensional Model for Prediction and Scale-up of Lyophilization
• Scale up of Fluid Mixing Parameters in Bio-Pharmaceutical Processes
• From Petrochemicals to Pharmaceuticals: Rapid Scale-up of Penicillin by an Academia-Industry Consortium Including Shell Development Company during World War II

### Synthetic Systems Biology II
***Hilton San Francisco, Plaza A***
• Optimizing Biological Circuits: Integrating Rational Design with Directed Evolution
• HIV's Evolution of Resistance to Antiviral Gene Therapy Is Predictable and Utilizes Novel Cooperative Mechanisms
• Engineering Ligand-Regulated RNAI Substrates as Novel Tools for Probing and Programming Cellular Systems
• Tunable Promoters for the Synthesis and Analysis of Functional Gene Networks
• Computational Design of Synthetic Biological Circuits
• Computer Aided Design of Modular Protein Devices: Logical "and" Gene Activation
• In Vitro Integration of Multiple Metabolic Systems for the Production of Membrane Proteins

### Thermodynamic Properties and Phase Behavior II
***Hilton San Francisco, Continental 6***
• Area 1a Keynote Address: Thermodynamics for the Design of Smart Surfactants and Ligands in Pharmaceutical, Environmental, and Energy Applications
• Phase Equilibria in the Ternary System of Carbon Dioxide–Tetrahydrofuran-Water at Gas Hydrate Forming Conditions
• Cosmo-Sac in Drug Design: Prediction of Partition Coefficients
• A Statistical Associating Fluid Theory for Electrolyte Solutions
• Condensed Phase Behavior of Benzene Using Monte Carlo Simulations
• Molecular Simulation of Three-Body Interactions on Vapor-Liquid and Solid-Liquid Phase Equilibria
• Extension of Scaled Particle Theory: Statistical Mechanics of Hard Sphere Pairs

### Transport at Interfaces II
***Hilton San Francisco, Union Square 23***
• Adsorption and Absorption of Polymeric Surfactants Onto and into Soft Contact Lenses
• Transport of Water and Ions across the Cunjunctiva and Its Effect on Ocular Tear Dynamics
• Flow Instability on Molecular Scale
• Modeling Transport and Kinetics of Crystal Growth from Solution
• Dynamics of Impact of Drops on a Substrate with Small-Scale Features
• Reflectivity Based Analysis of Contact Line Behavior and Microscale Heat Transfer in Binary Ultrathin Films
• Effects of Charge Discreteness on Electrostatic Interactions in Colloidal Dispersions
• Large Dynamic Contact Angles

### Utilization of DNA, Protein and Biological Cells
***Hilton San Francisco, Grand Ballroom A***
• Delivery of DNA, Proteins, and Cells with Injectable Hydrogels
• Bionanoparticles for Pinpoint Delivery of Genes and Drugs
• Engineering Modular Protein Polymer Vectors for Gene Delivery
• Protein-Mediated Synthesis of Uniform Superparamagnetic Magnetite Nanocrystals
• Bioimaging of Phosphorylation of ERK1 in Living Cell Using Fluorescence Resonance Energy Transfer
• Insulin Delivery from Genetically Modified Pancreatic Islets
• Use of Liposome Encapsulated Hemoglobin (LEH) as an Oxygen Carrier to Cultured Cells

### Water Quality Sensing and Detection Methods
***Hilton San Francisco, Imperial B***
• Biosensors for Environmental Monitoring
• DNAzyme-Based Nanosensors for Heavy Metals and Radionuclides
• Identification of Toxic Chemicals in Activated Sludge System by Denaturing High-Performance Liquid Chromatography
• Development of a Biosensor for Cryptosporidium in Drinking Water
• A New Hybrid Metal Oxide Particle as Sensor for Dissolved Heavy Metals

## MONDAY, 13 NOVEMBER 2006
***6:00 PM - 7:00 PM***
### SBE's James Bailey Award Lecture
***Hilton San Francisco, Grand Ballroom A***

## MONDAY, 13 NOVEMBER 2006
***6:30 PM - 9:00 PM***
### Engineering Education Poster Session
***Hilton San Francisco, Grand Ballroom B***
• The Use of a Simple Tank Level Process for the Illustration of Basic Control Concepts
• A Simple and Effective Strategy to Motivate Students When Teaching Technical and Economical Analysis in Engineering Programs
• Reconnecting Chemical Engineering Students with the Physical World
• Recruiting Middle School Girls to Engineering and Information Technology with Computer Mania Day
• Biochemical Extractions: Journal of Laboratory Reports
• Energy Requirement and Available Energy Consumption
• Thermo-Graphics: a Graphical Presentation of Chemical Engineering Thermodynamics Based on Mathematica, Karl B. Schnelle, Jr., Chemical Engineering Department, Vu Station B 351604, Vanderbilt University, Nashville, Tennessee, 37235-1604
• Developing Metacognitive Engineering Teams through Studying Learning Preferences
• Concept Mapping for Chemical Engineering
• Impulse: Innovative Process Design and How to Teach It
• Improving the Unit Operations Lab: Design Methods and Process Simulation as Basic Tools in the Distillation of Binary Mixtures
• A Fuel Cell Module for a Chemical Process Control Course
• Pivots: Service Learning at the Science, Theatre & Magic Boundary
• Student and Faculty Attitudes Towards Classroom Use of Tablet PCS

### Graduate Student Award Poster Session
***Hilton San Francisco, Grand Ballroom B***
• Carbon Monoxide Oxidation on Platinum Clusters Adsorbed on Pristine and Boron-Doped Carbon Supports: a DFT Investigation
• Optimization of the Solid-State Shear Extrusion Process for Low-Cross-Link-Density Natural Rubber with a Gaussian Slip-Link Model
• First Principles, Experiments, and Microkinetic Modeling of the Water-Gas-Shift Reaction on Pt(111)
• Polythiophene Forcefield Parameterization
• DFT Modeling of Electrocatalytic Reactions
• DFT Calculations of the Atomic Layer Deposition Growth Mechanisms of High-K Gate Dielectric Oxides
• *Ab Initio* and MD Studies of the Catalyst – Nafion Interfacial Region in PEM Fuel Cells
• Theoretical Study on Elementary Reactions in the Methanol-to-Olefin Process
• Nanoscale Structures, Breaking the Limits
• Parallel Monte Carlo Simulations through Sequential Updating Algorithms
• Effect of Confinement on Chemical Reactions
• Multiscale Modeling of Polystyrene in the Solution and in the Melt
• A Multiscale Approach for Phase Behavior, Structure and Macroscopic Properties of Colloidal Suspensions in Polymeric Fluids
• Force Field Development for 1,4-Dioxane and Molecular Simulation of Its Adsorption from Water
• Viscosity Calculation of Model Asphalt Mixture Systems

### Particle Technology Forum Poster Session
***Hilton San Francisco, Grand Ballroom B***
• Aggregation of Gold Nanoparticles: Experiments and Modeling
• Reducing Flame Spray Synthesis of Bismuth: Pure Metal Nanoparticles and Bulk Nanocrystalline Samples
• Release Profile of Phenanthrene into Coumarin Modified MCM-41
• Gas-Phase Synthesis of Pure Anatase Nanoparticles
• Nanoparticle Synthesis Using a Two-Stage Spray

Pyrolysis Generator
• Natural Coating, Protein Adsorption on Nanoparticles
• In Vitro Cytotoxicity Studies of Oxides Nanoparticles and Comparison to Asbestos
• Novel Nano-Particle Based Damping Systems
• Controlling the Interparticle Forces of Nanoparticles Using Atomic Layer Deposition
• Effect of Dry Particle Coating on Packing Density of Cohesive Powders under Low Consolidation
• Effect of Calcium Phosphate Nanoparticle on Osteoblast Survival
• Coating Variation at the Edge of a Tablet: an Experimental and Modeling Study of Droplet Impact Behavior
• Precipitation Using Carbon Dioxide as a Solvent in a Closed-Loop Thermosyphon
• Surface Modification of Cobalt-Substituted Ferrite Nanoparticles
• Design of an Electrochemical Adsorption Cell with under Control Particles Deposition
• Synthesis of Polyoxometalate Nanoparticles from Aqueous Foams
• An Experimental Investigation into the Effect of Moisture Content of Salt on Its Flow Properties
• Detailed Flow Modeling of Fluid Bed Processes in the Pharmaceutical Industry
• General Synthetic Route toward Functional Hollow Spheres with Double-Shelled Structures
• Voidage Wave Instability in a Vibrated Liquid-Fluidized Bed
• Formation Kinetics and Characteristics of Lead Sulfate Nanocrystals in Reverse Microemulsion
• Fluorescent Quantum Dot-Polymer Nanocomposite Particles for Biological Labels

**Pictures of Pilot Plants and University Unit Operation Labs**
***Hilton San Francisco, Grand Ballroom B***
• Pilot Plant for Distillation and Extraction Testing
• Pilot Plants for the Chemical Process Industry (2)
• The Ohio State University — Chemical Engineer Undergraduate Teaching Lab
• Unit Operations at the University of Illinois Urbana-Champaign
• Scale down: Unusual "Pilot Plants" and Unit Operations
• Abbott Laboratories Fermentation and Separation Pilot Plants
• The Undergraduate Laboratories at University of Notre Dame

**Poster Session: Interfacial Phenomena**
***Hilton San Francisco, Grand Ballroom B***
• Using Nanoparticles as Seeds for Nucleating Organic Nanorods
• Interfacial Behavior from First Principles
• Test-Area Simulation Method for the Direct Determination of the Interfacial Tension
• Controlling the Passage of Colloidal Particles across an Amphiphilic Membrane
• Drop's Line Energy as a Function of Drop Size – Resolving a Long Standing Puzzle
• One-Dimensional Simulation of Alkaline/Surfactant/Polymer Process for Enhanced Oil Recovery
• Rheological Behavior of Fluids with Microbubble Suspension and Surface Morphology of Microbubble Coating Materials
• High-Pressure Contact Angle Goniometry and Pendant Drop Tensiometry for the Design of Surfactants for the $CO_2$-Water Interface
• Biocompatible Surfactants for Dispersion-Based Pressurized Metered-Dose Inhalers
• Electrowetting of Water Droplet under an AC Electric Field
• Double-Carrier Systems as Novel Drug Delivery Vehicles
• Cracking in Wet Coatings of Aqueous Colloidal Dispersions
• Monte Carlo Simulations of Equilibrium Reactions Involving Charge Separation at a Vapor-Liquid Interface
• The Electrostatic Force between Dielectric Bodies
• Using NMR to Characterize Brine/Crude Oil Emulsion Formation and Stability
• A Molecular Approach for the Development of Hydrofluoroalkane-Based Pressurized Metered-Dose Inhaler Formulations
• Novel Nanosturctures of Polyaniline Via Interfacial Polymerization
• NMR Investigation of Polymerization-Induced Microphase Separation in Bis(Triethoxysilyl)Ethane
• The Motion of a Charged Water Droplet in Dielectric Fluid under Electric Field
• Critical Point of Electrolyte Mixtures
• Effect of Preparation Method on the Formation of Multilamellar Liposomes and Unilamellar Vesicles of Dilauroylphosphatidylcholine
• Controlling of Particle Interactions with Process Pipes in Calcite Mineral Processing to Prevent Depositions
• Direct Force Measurements for Analyzing Nanoparticle Stabilized Suspensions
• Investigating Model Peptides on Surfaces Using XPS, SIMS and NEXAFS
• Rapid Deposition of Nanocoatings and Wires from Aligned Tobacco Mosaic Virus
• Pattern Formation by Dip Coating and Evaporation of Colloidal Suspensions
• Advanced MVD Methods
• Charge Heterogeneity at the Crude Oil-Water Interface: a Probabilistic Study
• External Reflection-Absorption Ft-Ir Spectroscopy of HTAB, DTAB and C12e1 Molecules at Air/Water Interface
• Rheology of Bacterial Films at Hexadecane-Water Interface
• Formation of Rod-Shaped Calcite Crystals and Their Use as Templates for Silica and Titania Nanotubes
• A Branched Hybrid: Inducing Fatty Acid Nanorods from CdSe-MUA Nanoparticles
• A Novel Approach to Determine Critical Micelle Concentration of Surfactant Based on the First Derivative Treatment of Fluorescence Characteristics of Pyrene
• Novel Surface Coatings Using Electrostatic-Based, Controlled Multilayer Adsorption of Nanoparticles
• Predicting Diffusivity in Quenched-Annealed Systems

**Poster Session: Materials Engineering and Sciences Division**
***Hilton San Francisco, Grand Ballroom B***
• Tuning Pore Size of Mesoporous Carbon Via Confined Activation Process
• Plasma-Radiation Enhanced Nanofiber-Thermoplastic Composites
• Preparation and Characterization of Organic-Inorganic Nanostructured Hybrid Coatings
• Conductive Polythiophene/Zeolite Composites as CO and $SO_2$ Sensors
• Modeling of Chain Sequence Distribution in Thermoplastic Condensation Terpolymers
• The Application and Modeling of Nano-Structured Polymeric Liquid Films in Head-Disk Interface
• Gelation, Pore Structure, and Ionic Conductivity in Silico-Phosphate Proton Exchange Glass Membranes
• Molecular Simulations of Chemically Crosslinked Polyelectrolyte Networks in Salt Solutions
• Production of Molybdenum and Tungsten Carbide Ultrasonically Dispersed Nanocrystallites
• Combinatorial Study of Polyvinylidene Fluoride Network Membranes for PEM Fuel Cells
• Preparation of Highly Catalytically Active Cu/Zno and Cu/Zno/$Al_2O_3$ Materials by Metal-Organic Chemical Vapor Deposition
• Synthesis of Complex Hydride Reversible Hydrogen Storage Materials
• Advances in Military Coatings Systems
• Adsorption of Dibenzothiophene and Its Alkyl Derivatives in Polymers Containing Hydroxyl and Amino Groups
• Synthesis, Characterization, and Properties of Flexible Side-Chain-Containing Polyimides
• Effect of Salt on Gold Nanoparticles Formation in PEO-Pp-PEO Block Copolymer Solutions
• Poly(Ethylene Glycol)-B-Polycaprolactone Nanoparticles and Their Use as Drug Delivery Vehicles
• Conductivity and Gas Sensing Properties of Nanocluster Iron Oxide Aerogel
• Self-Assembly in the Formation of Mesoporous Silica Aerosolized Particles Containing Fluorescent Polymers and Drugs for Sensor and Controlled Release Applications
• Surface Modification of Deep-Grooved Fibers Using Hydrophilic Migratory Additives
• Studying Different Factors on Corrosion of Coated Titanium Anodes in a NaCl Solution
• The Kinetics of Reducing End-Specific Exo-Acting Cellobiohydrolases
• Surface Coverage, Structure, and Hybridization Behavior of Mixed DNA/Alkylthiol Monolayers on Gold
• Investigation of Corrosion with Material Selection in Flue Gas Desulfurization & Waste Incineration Systems
• Investigation of Corrosion of Reinforcement Concrete with Different Pozzolans in the Sour System
• Controlling Diffusion Properties of Peg Hydrogels by Varying Polymerization Characteristics
• Altering the Mechanical Properties of Protein-Based Polymers
• Gas Barrier Properties of Polymeric Films with Hybrid Organic/Inorganic Coatings
• Temperature-Sensitive Copolymers of *n*-Isopropyl-Acrylamide and N,*n*-Dimethylacrylamide: Application in Hyperthermia-Directed Gene Delivery
• Swelling Behavior of End-Linked Pamam-Peg Hydrogels
• Preparation of Ni-Supported Mesoporous Silica by Intercalation Treatment
• Synthesis of Mesoporous Tio2 Particles Using Replication from Mesoporous Silica Materials
• Nanoscale Morphology of Ionomer Systems
• The Effects of Different Silanes and Metal Surface Treatments on the Binding of Chitosan as Investigated by Mechanical and Biological Testing
• Viscoelastic Scaling, Bubble Nucleation and Growth in Microcellular Extrusion Foaming of a Polystyrene Carbon-Dioxide System
• Curing of Montmorillonite Modified Epoxy-Polysulfone Blends
• Responsive, Cross-Linked Layers Based on Benzophenone-Modified Poly-(*n*-Isopropylacrylamide) Polymers
• Absorption and Diffusion in Bio-Based Polymer Films
• Template Synthesis of Mesoporous Tin Oxide with High Thermal Stability
• New Synthetic Route for the Incorporation of Au Nanostructure (Particles and Wires) into the Pores of MCM-41
• Luminescent Mesostructure Lanthanide Complex/Silica Nanocomposites Via Assembly of Bridged 2, 6-Diaminopyridine Silsesquioxanes
• Dispersions of Core-Shell Dielectric Nanoparticles and the Optimization of Uv Scattering and Absorbance to Minimize the Transmittance of Novel Sunscreen Materials
• The Enhanced Barrier Effects and Thermal Properties of Polymer/Alumina Nanocomposites Fabricated by Atomic Layer Deposition
• Novel, High-Strength Nanostructured Composites Prepared with Layer-by-Layer Assembly Technique
• Development and Characterization of Magnetorheological Elastomers
• Assessment of the Biological Stability of Hemoglobin I from Lucina Pectinata and Myoglobin from Horse Skeletal Muscle in Ionic Hydrophilic Polymer Networks
• The Effect of Processing Variables on the Rate of Water Absorption by Wood Plastic Composites
• Composite Materials of Thermo-Responsive Polymer Networks and Inorganic Nanoparticles
• Study of the Effects of Halogenated and Non-Halo-

genated Flame Retardants on Flammability of Acrylonitrile-Butadiene-Styrene (Abs)/Wood Composites
• Study of Water Adsorption on Activated Carbon with Different Surface Oxygen Complexes
• Computational Study of Zno Deposition from Diethylzinc and Water in Metal Organic Chemical Vapor Deposition
• Electrochemical Capacitor Behavior of RuO2 Vertically Aligned Rods Filled with RuO2•XH2o
• Shear-Induced Structure & Rheology of a Polymeric Sponge Phase
• Synthesis of Periodic Mesoporous Materials from Various Zeolites
• Precise Particle Size Control of Large Pore Mesoporous Silica in Nanoscale
• Preparation of Mesoporous Metal Oxides by Nano-Replication Route Using Mesoporous Silica as Template
• Effect of Compatibilizer Blends on Mechanical and Thermal Properties of HDPE/Wood/Clay Nanocomposites
• Linac Electron Beam Irradiation of Carbon Nanotubes: Functionalization and Characterization
• Dispersion of Surface-Functionalized Multiwalled Nanotubes into Nanostructured Polymer Networks: Synthesis and Characterization
• Segmental Relaxation Characteristics of Rubbery Membrane Networks
• Mechanical Oscillating PNIPAM Gel Particles
• Examination of the Effects of Poly(Ethylene Glycol) (Peg) Rich Matrices on the Transport of Multi Drug Resistance (MDR) and Multi Drug Resistance Associated Protein (MRP) Substrates Utilizing the CaCO-2 Cell Model
• Adhesion Strategy of Homo- and Hetero-Polymers
• Studies of Ferrite Based Magnetic Nanoparticle Transport Mechanisms and Magnetocytolysis Effects on a Model Cell Cultures
• Measurement of the Infinite Dilute Activity and Diffusion Coefficients of Small Molecule Solvents in Cross-Linked Polyvinyl Alcohol by Inverse Gas Chromatography
• Development of PPV/Zeolite Composites for Co Sensor
• Development of Polythiophene/Zeolite Composites as $H_2$ Sensor
• Development of Polymer Blend between Poly(P-Phenylene) and Acrylic Elastomer for Electroactive Application
• Characteristics and Deposition Kinetics of Electroless Nickel-Tungsten-Phosphorus Alloys Plated from Slightly Basic Bath
• Islet-Derived Cell Aggregates for Encapsulation
• Recyclability of Flame Retardant Polycarbonate: Comparison of Non-Halogenated to Halogenated Flame Retardants
• High-Yield Approach of Zeolite Nanocrystal Synthesis
• Surface Modified Magnetorheological Elastomers – Oxidative Stability
• Effects of Reactive Microgels on the Volume Shrinkage for Low-Temperature Cure of Unsaturated Polyester
• Effects of Additives on Rheological Properties, Atomization, and Coating Strength of Polyethylene Oxide Aqueous Solution
• Announcement of Student Poster Winners (End of Session)
• A Comparison of Rheological and Structural Properties of Linear Polyethylene Melts under Shear and Elongation Flow Using Nonequilibrium Molecular Dynamics Simulations
• A Novel Antibacterial Polymer: Orthopedic and Other Applications

**Poster Session: Nanoscale Science and Engineering**
***Hilton San Francisco, Grand Ballroom B***
• Modeling of Transport through Nanocomposite Membranes
• On the Origin of a Permanent Dipole Moment in Cubic Nanocrystals
• Aqueous-Core Capsules Via Direct Interfacial Polymerization
• Cobalt Nanoparticles by Reducing Flame Synthesis
• Release of Gold Nanoparticles from Phytomined Biomass by Enzymatic Digestion
• One-Pot Synthesis of Hierarchically Structured Metal Oxides
• Synthesis and Applications of Thin Ceramic Films with Oriented Nanopores Formed by Evaporation-Driven Self-Assembly
• Generation of Kinetic "Phase Diagrams" for Self-Assembled Nanopattern Formation in Heteroepitaxy Via Hierarchical Multiscale Modeling
• Controlling the Quantum Wire Quality in Crystalline Titanosilicates ETS-4 and ETS-10
• Europium Doped Yttrium Oxide Nanoparticle-Silica Composite as an Energy-Efficient Phosphor Material
• Study of Recognition between Bacteria and Antibody Molecules on Peg Tethered Silicon-Based Biosensors by Atomic Force Microscopy
• Nanomechanical Property Measurement of Superoxide Dismutase Aggregates Via an Atomic Force Microscope Tip-Induced Molecular Pulling
• Direct Force Balance Method for AFM Lateral Force Calibration
• Fabrication of Polypyrrole Nanotubes Using Electrospun Hydrophobic Polymer Nanofiber Templates
• Ab Initio Band Structure Studies of Pristine Silicon Nanowires
• Pore Expansion in Fluorinated and Hydrocarbon Surfactant Templated Silica Thin Films Due to Supercritical Carbon Dioxide Processing
• Determination of the Magnetic Anisotropy Constant for Magnetic Nanoparticles Using a Debye Model
• Synthesis and Growth Kinetics of ZnS and CdS Quantum Dots Via Reverse Micelles
• Rheological Studies of Nanoparticle Embedded Linear Chain Polymer under Shear Using Molecular Dynamics Simulations
• Dendrimer-Directed Synthesis of Shell Cross-Linked Nanocages with Amine Interior Walls
• Surface Modification of Magnetite ($Fe_3O_4$) Nanoparticles for Cancer Treatment
• Dendrimer-Assisted Low-Temperature Growth of Carbon Nanotubes by Plasma-Enhanced Chemical Vapor Deposition
• Effects of Surface Properties on Solid-Supported Two-Dimensional Protein Crystals
• Simcell: Simulation of Discrete Nanoscale Transport in Cells
• Temperature Profile in the Oscillatory Behavior of Double-Walled Carbon Nanotubes
• High Aspect Ratio Uv-Nano-Embossing Using a Novel Low Cost Nano-Mold Fabrication Technique
• Oriented Composite Mesostructures under Nanoscale Confinement
• Non-Linear Deformation of Tethered Sio2 Nanocomposites
• Influence of Chaotic Mixing on Morphology and Rheological Property of Polypropylene/Nano-Calcium Carbonate Composite
• Nanobumps Created with Polystyrene Spheres and 248nm or 308nm Laser Pulses

**TUESDAY, 14 NOVEMBER 2006**
***8:30 AM - 11:00 AM***
**(22b) Nanotechnology and Nanobiotechnology for Sensors I**
***Hilton San Francisco, Plaza B***
• Electrochemical Sensor for Toxic Chemicals Based on Nanodeposit and Enzyme
• Nanostructured Biosensor for Detecting Neuropathic Agents
• High Density Microchip Biosensors Using Intact Liposome Arrays
• Controlled Assembly of Multi-Component Nanowires by DNA Hybridization
• Highly Sensitive Biomolecular Fluorescence Detection Using Nanoscale Zinc Oxide Platforms
• Electrical Characterization of Lipid Membrane Supported Onto Silicon Nanowires
• Carbon Nanotube Complexes for the Selective Detection of DNA Sequences

**Advanced Oxidation Processes**
***Hilton San Francisco, Union Square 14***
• Enhancement of Photcatalytic Mineralization of Phenol in the Presence of Ferric Ions: Kinetic Modeling and Parameter Estimation
• Free Radical Chemistry as the Underpinning for Advanced Oxidation Processes
• Use of Pulsed Corona Discharge Reactors (PCDR): Results for Protein Degradation in Aqueous Phase
• Electrochemical Oxidation and Mineralization of Acetaldehyde
• Anodic Oxidation of Wastewater Constituents; Investigation of Process Parameters
• Advanced Oxidation Processes; the Role of the Redox Couple Fe+3/Fe+2
• Evaluation of Chemical Oxidizer-Soil Interactions and Their Impact on the Efficiency of in situ Chemical Oxidation

**Advances in Electrokinetics and Electrophoresis - Particles and Biomolecules**
***Hilton San Francisco, Yosemite A***
• Electrolyte Dependent Aggregation or Separation of Micron Sized Particles in Low Frequency AC-Electric Fields
• Isotachophoresis: from Grams to Nanograms
• Use of Photopolymerized Sol-Gel for Chemical Analysis
• Potential Pathogen Destruction Technique: Reduction of Vibrio Parahaemolyticus Viability in a Dielectrophoretic Field
• Numerical Simulations of Electrokinetically-Driven Capture of Viral Particles inside Media of High Ionic Strength
• Effect of Electro-Advective Based Flows on Optimal Separation Times for Biomacromolecules

**Advances in Liquid Separation Membranes and Applications**
***Hilton San Francisco, Yosemite B***
• Interfacially Polymerized Thin Film Composite Membranes Based on Microporous Polypropylene Hollow Fibers
• Nano-Structured Compaction Resistant Thin Film Composite Membranes
• Methodological Assessment of Nanofiltration Membrane Performance Based on Surface Properties
• Controlled Graft Polymerization as a Tool for Membrane Surface Modification
• Cleaning of Reverse Osmosis Membranes Fouled by Combined Organic Foulants
• The Development of Chemically Modified P84 Co-Polyimide Membranes for Cu(II) Removal Using Supported Liquid Membranes with Prolonged Stability
• Concentration of Single-Cell Dunaliella in Solution and Recycle of Nutrient Components from Algal Residue by UF

**Advances in Protein Engineering (I)**
***Hilton San Francisco, Continental 7***
• Understanding the Reaction Mechanism of Protein Splicing in Order to Gain Insights for the Engineering of Interns
• Antibody Affinity Maturation Using Computational Protein Design
• Computation-Guided Design of Arac Regulatory Protein Effector Specificity
• Application of the Consensus Concept for Increased Thermostability of Enzymes
• A General Method to Directly Improve Kinetic Stability of Enzymes without Reducing Activity
• Engineering Transcription Factors with Novel DNA-Binding Specificity Using Comparative

Genomics
• Genetic Selection of Stable Single-Chain Immunotherapeutics in the Cytoplasm of *Escherichia Coli*

### Artificial Organs, Bioreactors and Disease Modeling
***Hilton San Francisco, Continental 3***
• Network-Based Mechanistic Model for Tumor Growth Development
• Modeling of Endovascular Coil Embolisation of Cerebral Aneurysms
• Origami - the Retrosynthesis of Organ
• Cells Culture in Perfusion Bioreactors: Analysis and Selection of Scaffold Channelling Structure Based on Reynolds and Peclet Numbers
• Three-Dimensional Cell Seeding and Culture in Novel Radial-Flow Perfusion Bioreactor
• A Porous Perfusion Bioreactor That Possess Microchannels: Its Fabrication by Selective Laser Sintering and Preliminary Value of Culture of Human Hepatoma Hep G2 Cells
• Kinetics of Nitric Oxide Interactions with a Cysteine-Modified Polymer

### Biomaterial and Scaffold Design for Tissue Engineering
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Biodegradable and Photopolymerizable Hydrogels for Tissue Engineering Application Based on Poly(Ethylene Glycol) and Diacid Monomers
• Biodegradable Fumarate-Based Polyhipes as Tissue Engineering Scaffolds
• Mechanically Stimulated Photopolymerized Hydrogels for Cartilage Tissue Engineering
• Recent Progress on Developing Advanced Methods and Materials for Fabricating Hierarchically Structured Tissue Engineering Scaffolds Using Stereolithography
• Three-Dimensional Neuronal Culture on Inverted Colloidal Crystal Hydrogel Scaffold Modified with Layer-by-Layer Assembled Single-Wall Carbon Nanotubes
• Development of Microvascularized Tissue-Engineered Products: Flow Characterization and Scaffold Fabrication
• Multiple Channel Bridges Releasing Bioactive Factors to Promote Spinal Cord Regeneration

### Biomolecules at Interfaces III - Engineered Interfaces for Implants and Sensors
***Hilton San Francisco, Union Square 22***
• Polymer Brush Layers with Variation of Grafting Density for Peptide Adsorption and Cell Adhesion Studies
• Understanding the Non-Fouling Mechanism by Paired Experiments and Simulations
• "Clicking" Biomolecules Onto Alkyne-Functionalized Surfaces
• Dynamics of Novel Multifunctional, Intelligent Mucoadhesive Copolymers
• Peptoid Analogues of Lung Surfactant Protein C
• Toward Label-Free Electrochemical Sensing of Nucleic Acids
• Detection of Antibody Binding to a Tethered Vesicle Assembly Using QCM-D
• Thermally Induced Conformational Changes in Macromolecules Detected on a Microcantilever Surface
• Reactions of Amino Acids on SiB and Ge Surfaces

### Building Drug Delivery into Tissue Engineering
***Hilton San Francisco, Continental 8***
• DNA Loaded Multiple Channel Bridges for Spinal Cord Regeneration
• Microfluidic Scaffolds for Tissue Engineering
• Enhancing Nanoparticle Penetration in the Brain by Convection Enhanced Delivery and Enzymatic Degradation of the Extracellular Matrix
• Calcium Phosphate Shell Delivery System for Bone Repair
• Osteoblast Response to Amorphous Calcium Phosphate *in Vitro*
• The Hydroxyapatite Affinity and Binding Kinetics of Peptides Modified with Bisphosphonates, Poly(Aspartic Acid), and Poly(Glutamic Acid)
• Affinity Hydrogels: Tailored Protein Delivery from Permissive Tissue Engineering Matrices

### Case Studies in Product Design - I
***Hilton San Francisco, California Room***
• Engineering Skin Lotions
• A Modeling Strategy for Optimal Solvent Composition Selection in the Design of a New API Process
• Property Clustering Techniques for Experimental Design
• Development of Web-Based on-Line Optimization System
• Development of Fats and Oils Blend Using Case-Based Reasoning
• A Systematic Property Clustering Approach to Molecular Design

### Catalysis with Microporous and Mesoporous Materials I
***Hilton San Francisco, Franciscan C***
• Kinetics, Mechanism, and Structure Requirements for Selective Terminal Oxidation of Linear Alkanes on Mn-Modified Microporous Catalysts
• The Role of Surface Modification of Mesoporous Silica on the Reactivity and Stability of Supported Au
• Dealuminated Y Zeolite-Supported Mononuclear Iridium Complexes with Reactive Ethylene Ligands: Synthesis, Characterization, and Catalysis of Ethylene Hydrogenation
• Stability and Reactivity of Re- and Mo- ZSM5 Catalysts for $Ch_4$ and $C_3h_8$ Conversion
• Aromatization of *n*-Octane over ZSM-5 Zeolite Catalysts and Its Reaction Pathways
• Solid Acid Porous Catalysts for the Transformation of 1-Adamantanol
• A Novel Approach for Preparing Heterogenized Homogeneous Catalysts in Mesoporous Polymer Supports

### Colloidal Assembly and Fabrication
***Hilton San Francisco, Union Square 24***
• Engineering Novel Colloidal Crystal Structures Using DNA-Mediated Self-Assembly
• Programmed Self-Assembly of a Biosensor to Probe Cell Adhesion Interactions
• Columnar Self-Assembly of Nanodisks
• Properties of Surface-Anisotropic Polystyrene Particles
• The Controlled Synthesis of Complex Microparticles Using Continuous Flow Lithography and Their Self-Assembly
• Shape Selectivity in the Assembly of Lithographically-Designed Particles
• Unexpected Correlations Observed in Two-Dimensional Ordered Arrays of Colloidal Particles Deposited on Patterned Polyelectrolyte Multilayer Surfaces

### Colloidal Dispersions I - Interactions & Assembly
***Hilton San Francisco, Union Square 25***
• Surface-Induced Attraction between like-Charged Particles at the Oil-Water Interface
• Jamming and Melting in Colloidal Suspensions of pH-Responsive Hydrogels
• Impeded Dynamics of Colloidal Suspensions under Confinement
• Colloidal Interactions at an Oil-Water Interface
• Engineered Assembly of Uniform Hierarchically Porous Patches from Metal Nanoparticles
• In-Suspension Fabrication of Multi-Material Colloidal Doublets
• Imaging Interfacial Energy Landscapes with Concentrated Diffusing Colloidal Probes

### Combustion Reaction Engineering
***Hilton San Francisco, Imperial A***
• Reduction Kinetics of COo-NiO/Al2o3 Oxygen Carrier for Chemical-Looping Combustion
• Comparative Evaluation of Novel Oxygen Carriers for Chemical Looping Combustion
• Larger Unsaturated Radicals under Combustion Conditions
• Hydrothermal Flames in a Novel Supercritical Water Oxidation (SCWO) Reactor
• Three-Dimensional Microscale Numerical Simulation of Smoldering
• Modeling Evaporation and Microexplosion of Water-in-Alkane Emulsion Droplets
• Ignition Mechanisms of Metal-Coated Aluminum Particles

### Complex-Fluid and Bio-Fluid Dynamics I
***Hilton San Francisco, Union Square 15 & 16***
• Flow of Polymer Solutions in Nonuniform Channels
• Bead-Rod Simulation of DNA Dynamics in Converging/Diverging Micro/Nanofluidics
• Trapping Pathogens with Secondary Stagnation Flows
• Hydrodynamic Interactions in Semidilute DNA Solutions in Microfluidic Flow
• Ergodicity-Breaking and Glassy Dynamics in the Stretching Flows of Single Polymer Molecules
• Dynamics of Macromolecules in Two-Dimensional Linear Flows with Rotation: Is There Another Coil-Stretch Transition?
• DNA Dynamics in Nanofluidic Channels
• Near-Contact Motion of Deformable Surfactant-Covered Drops
• 3-D Imaging of Unsteady Fluid Flow in Microchannels
• Sagging and Hoisting of a Viscoelastic Filament

### Composites I
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Mechanical Studies of Cellulose Nanocrystals-Polymer Composite Thin Films
• Novel Approach for Joining Carbon-Carbon Composites Using High-Temperature Heterogeneous Combustion Reactions
• Preparation, Structure, and Properties of Nanoparticles and Long Fibers Reinforced Thermoset Composites
• Modeling of Polymer Melts Containing Short and Long Glass Fiber. Part II: the Simulation of Injection Molded Parts
• Interlayer Toughening of Vinyl Ester Matrix Composites Using Electrospun Nano- and Meso- Fibers
• Experimental Investigations of the Protection Capabilities of Novel Chemical Protective Substrates
• Environmentally Friendly Polymers and Composites for Military Applications

### Developments in Thermochemical and Electrolytic Routes to Hydrogen Production: Part III
***Hilton San Francisco, Taylor***
• Evaluation of Alternate Thermochemical Cycles
• A New Methodology to Screen Water Splitting Cycles for Hydrogen Production
• An Algorithm for Systematic Generation of Thermochemical Cycles for Water Splitting
• Application of a Process Model-Free Analysis to Thermochemical Systems for Large-Scale Hydrogen Production
• Reaction Kinetics of the High Temperature Zno Dissociation Step in a 2-Step Solar Thermochemical Water Splitting Process
• Investigation of the Water Reduction with Zinc Powder Aerosol to Form Hydrogen Fuel

### Disease Therapies and Diagnostics
***Hilton San Francisco, Continental 9***
• An Injectable Polymeric Device for Drug Delivery and Sensing
• Application of Immunomagnetic Cell Enrichment in Combination with Rt- Pcr for the Detection of Rare Circulating Cancer Cells in Peripheral Blood and Bone Marrow from Patients with Head and Neck Squamous Cell Carcinoma (HNSCC)

• Cd4+ T-Cell Epitope Identification Using Yeast Displaying Single Chain Class II Mhc Molecules as Artificial Apcs
• Detection of Active Amyloid-Beta Species Using a Quartz Crystal Microbalance
• Development of Novel Sialic Acid Containing Polymers for Use in Alzheimer's Disease
• Assessment of Islet Quality
• Metabolic Re-Engineering for Obesity Drug Target Identification: Flux Analysis and Gene Profiling of Forced Uncoupling Protein 1 Expression in 3t3-L1 Cells

### Distillation Honors: Zarko Olujic I
***Hilton San Francisco, Plaza A***
• Academia and Industry: a Perpetual Marriage for Distillation
• Separation Efficiency Estimation without Mass Transfer Coefficients: a New Approach for Structured Packed Columns
• Modeling the Hydrodynamics of Last-Generation Catalytic Structured Packings
• Trays or Packing for Acid Gas Absorbers?
• Towards the Practical Application of the Internally Heat-Integrated Distillation Columns (HIDIC)
• Mass Transfer Performance of an Annular Heat Integrated Sieve Tray

### Engineering of Novel Therapeutic Devices
***Hilton San Francisco, Continental 1***
• Blends of L-Tyrosine Based Polyurethanes and Polyphosphate for Biomedical Applications
• Reversible Modulating Gels Via Tertiary Conformation Switching of RNA Motifs
• Skin-Cad®: Pharmacokinetic Model for Transdermal Drug Delivery
• In Vitro Investigation of Oral Insulin Delivery Systems Using Lectin Functionalized Complexation Hydrogels
• Microdermabrasion of Skin for Drug and Vaccine Delivery
• Rapid Drug Microadministration toward Neuron Using Electrochemical Micropump for Brain Therapy
• Novel Alternating Copolymer Structures for Targeted in Vivo Imaging and Therapy in Cancer

### Fundamental Research in Transport Processes I
***Hilton San Francisco, Union Square 21***
• Transport and Spatial Pattern of Intracellular Organelles
• Theory and Experiments for the Surfactant Adsorption from Micellar Solutions Onto an Initially Clean Air/Water Interface: Evidence of the Direct Micelle Adsorption Route
• Driving Force for Molecular Diffusion: Comparision between Theory and Simulation
• Multicomponent Diffusion: Tests of Existing Theories
• Small Molecule Diffusion in Semicrystalline Polymers
• Dispersion in Porous Media for Multicomponent Systems
• Diffusion of a Single Polymer Chain in Colloidal Suspensions in Narrow Channels
• A New Kinetic Model for Gas Hydrates Using Collision Theory

### Fundamentals of Environmental Catalysis I
***Hilton San Francisco, Franciscan B***
• Conversion of Hydrogen Sulfide in Coal Gases to Liquid Element Sulfur and Gaseous Carbonyl Sulfide
• Formation of Liquid Element Sulfur and Carbonyl Sulfide by Oxidizing Hydrogen Sulfide in Coal Gases
• Interactions of Sulfur with High Surface Area Carbides and Nitrides
• Cleanup of Coal Gases by Removing Hydrogen Sulfide in the Form of Liquid Element Sulfur
• Titania-Based Nanocomposite Materials as Highly Active Photocatalysts
• Polyols and Organic Acids Adsorption Onto Activated Carbon, and Its Role on Aqueous-Phase Catalytic Hydrogenation Rates
• Selection of an Efficient Catalyst for the Catalytic Wet Air Oxidation of Orange II: a Mono Azo Dye
• Impact of Electrode Surface Morphology on the Electrochemical Reduction Kinetics of Nitroaromatics and Cyclic Nitramines Mixtures
• Electrocatalytic Dechlorination of 2-Chlorobiphenyl at a Palladium Modified Granular-Graphite-Packed Electrode

### Fundamentals of Fluidization I: in Honor of Prof. Bob Pfeffer on the Occasion of His 70th Birthday
***Hilton San Francisco, Franciscan D***
• Packing, Fluidization, and Other Applications of Cabot Nanogel®
• Material Bridges between Small Particles in a Powder: Application to Sticking, Caking and Granulation
• Heterogeneous Model for the Adsorption and Reaction on the Surface of Highly-Agglomerated Nanoparticles in a Fluidized Bed
• Fundamental Particle Fluidization Mechanism and Handling of Fine Particles in a Rotating Fluidized Bed
• Surface Roughness in Free-Surface Flow of Concentrated Suspensions
• Filtered Two-Fluid Models for Gas-Particles Flows
• Wave Propagation and Granular Temperature in Fluidized Beds of Nano and FCC Particles

### Fundamentals of Interfacial Phenomena I
***Hilton San Francisco, Union Square 13***
• Biomimetic Superhydrophobic Silicon Surfaces
• Effect of a Nanoporous Surface on Wettability of an Evaporating Meniscus
• Modeling Interfacial Behavior in Complex Porous Materials
• Fundamental Understanding of Adsorbed Water on Silicon Oxide
• Molecular Dynamics Simulations of Hydration Force in Aqueous Solutions Confined between Mica Surfaces
• Static and Hydrodynamic Interaction Forces between Pluronic Stabilized Emulsion Droplets Measured Using AFM
• Dynamic Wetting and the Encapsulation of Voids in Free Surface Flows

### Fundamentals of Nucleation
***Hilton San Francisco, Lombard***
• Critical Supersaturation in Solution Crystallization as a Function of Equilibrium Cluster Size Distribution
• Affecting Polymorph Selectivity in a Reproducible Nucleation Environment Generated Using a Microfluidic Device
• Controlling Hydroxyapatite Nucleation from a Simulated Body Fluid
• Crystal Nucleation in Polymorphic Systems: Effect of pH, Supersaturation and Molecular Speciation of Impurities
• Directing the Crystallization of a Desired Polymorph through Secondary Nucleation (Seeding)
• Examination of Crystal Nucleation and Polymorph Transitions through Molecular Dynamics Simulations of Hard-Core Screened Coulomb Particles
• Role of Solubility Enhancers in Protein Crystal Nucleation and Growth

### Injectable Biomaterials
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Novel Thermally Responsive Macromers for the Fabrication of Injectable, *in Situ* Crosslinkable Hydrogels
• Rapidly Setting Calcium Phosphate Cements Based on Amorphous Tricalcium Phosphate Nanoparticles
• Evaluation of Novel Injectable Hydrogels
• Biodegradable, Injectable Poly(Ester Urethane)Urea Delivery Systems for Bone Tissue Engineering
• A Novel Injectable Polymeric Biomaterial Poly(Propylene Fumarate-*Co*-Caprolactone) with Controllable Properties for Bone and Nerve Regenerations
• Thermal Gelation and Phase Equilibria of Responsive Elastin-Mimetic Triblock Hydrogels
• Modeling and Gelation Kinetics of Injectable in Situ Crosslinkable Poly(Lactide-Ethylene Oxide-Fumarate) Hydrogel Networks

### Intellectual Property Issues in University-Industry Collaborations
***Marriott San Francisco, Pacific I***
• Best Practices in Protecting Intellectual Property Issues
• Finesse Intellectual Property Issues in Sponsored Research Agreements
• Patent Strategy in the Context of United States Patent Reformation
• Recent Patent Disputes and Implications for Collaborations: What Can Be Done Better?

### Interfacial Flows II
***Hilton San Francisco, Union Square 17 & 18***
• Hysteretic Rheological Response of a Highly Viscous Drop in Linear Flows with Rotation
• Finite-Amplitude Capillary Oscillations of Coupled Droplets
• Instabilities and Saturation of Electrified Thin Liquid Films
• A Multi-Scale Polymer Foam Model and Its Application
• Continuum Modeling and Flow Visualization of Blown Foams
• Experimental and Modeling Studies on Solitary Wave Dynamics on Vertical and Inclined Film Flows
• Slip and Air-Entrainment at Water-Solid Interfaces
• The Impact of Fluid Behavior on the Wedge-Flow near Moving Contact Lines
• AC Electrospraying: Quasi-Steady Cones and Microjets
• A Microscopic View of Liquid-Liquid Film Flows

### Laminar Mixing and Mixing Fundamentals
***Hilton San Francisco, Mason***
• Experimental and Correlational Studies of a Vickers-Zimmer Style Polyester Finisher
• Experimental Investigation of Non-Newtonian Mixing with the Maxblend Impeller
• Performance of a Dual Shaft Mixer for Gas-Viscous Liquid Processing
• Measurements and Simulation of Flooding Characteristics for Gas-Sparged Stirred Vessels with Highly Viscous and Viscoelastic Liquids
• Impact of the Unstable/Neutral Angle on Rate and Extent of Chemical Reaction
• Menagerie of Topology in 3d Steady Flow

### Life Cycle Assessment and Sustainability Metrics
***Hilton San Francisco, Continental 6***
• Life Cycle Assessment of Mobile Telephones Based on Greenhouse Gases and Electricity Consumption
• Philosophical Background of Green and Sustainable Chemistry and Its Metrics in Japan
• Life Cycle Inventory - the Quality of Inputs
• Thermodynamic Life Cycle Assessment of Emerging Technologies
• New Stochastic Simulation Capability Applied to Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (Greet) Model
• Sustainability and Life Cycle Principles in Practice: GlaxoSmithKline's Experiences with FLASC Tm (Fast Life Cycle Assessment of Synthetic Chemistry)
• Multiple Criteria Decision Making for Sustainable Chemical Process Design
• Control Theory Applications for the Life Cycle Assessment of Improved Industrial Sustainability

### Membranes for Bioseparations I
***Hilton San Francisco, Continental 2***
• Effects of pH and Ionic Conditions on Microfiltration of Mammalian Cells: Combined Permeate Flux Enhancement and Mab Purification Capabilities
• Improving Permeate Flux in the Microfiltration of a Bacterial Cell Suspension by Flocculation with Cationic Polyelectrolytes

• Protein Fouling of Microfiltration Membranes in in-Line Modules
• Nature-Inspired Protein Adhesion-Resistant Membranes
• Organic-Inorganic Hybrid Membranes for Protein Purification
• Viral Filtration of High-Titer Mab Solutions with Hollow Fiber Membranes
• Virus Capture by Tangential Flow Filtration

### Nucleation and Growth
***Hilton San Francisco, Union Square 3 & 4***
• The Influence of Critical Cavities on Homogeneous Bubble Nucleation: a New Picture of Bubble Formation?
• Effects of Geometric Defects on Superheated Heterogeneous Bubble Nucleation: Molecular Dynamics Study
• Simulation of Gas-Liquid Homogeneous Nucleation: a Molecular Dynamics Study
• Monte Carlo Simulation of the Crystallization of Isotactic Polypropylene
• Nucleation of Colloidal Crystals Via Emulsion Crystallization
• Polymorph Selection during Crystal Nucleation and Growth
• Nucleation and Crystal Growth of Insulin as a Fundamental Mechanism of Regulation in Mammalian Organisms

### Pilot Plants in the Food and Consumer Products Industries
***Hilton San Francisco, Van Ness***
• Pilot Plants: Scaling down from Commercial Production Plants
• Unique Pilot Plant Capabilities in the Canadian Prairie
• Food and Chemical Pilot Plants – What Are the Differences?
• Using Pilot Plants Creatively to Reduce Product Development Cycle Time
• Re-Use of Pilot Plants to Meet Consumer Products Feedstock Demands

### Plenary Session II on Membranes and Bioseparations Honoring Professor Ed Lightfoot
***Hilton San Francisco, Continental 5***
• Searching for Oligomers during Insulin Fibrillation
• Biocatalysis and Ion Separation with Pore Assembled Polypeptide Multilayers in Membranes
• Electrostatic Interaction Chromatography for Separation of Very Similar Proteins – Effects of Stationary and Mobile Phase Properties
• Strategies for Super-Hydrophobic Surface Design
• Biomolecular Interactions at Phospholipid-Decorated Interfaces of Thermotropic Liquid Crystals
• Metal Affinity Separations of Nucleic Acids

### Polymer Membranes for Gas Separations
***Hilton San Francisco, Yosemite C***
• $CO_2$ Separation Using Nanocomposite Membranes Made of Bromine Modified 2,4-Dimethyl-1,6-Phenylene Oxide and Chemically Modified Silica
• Polymeric-Metallic Composite Membranes for Hydrogen Purification and Carbon Capture at Elevated Temperature
• The Diamine Modification of P84 CO-Polyimide Membranes for Pervaporation Dehydration of Isopropanol
• Formation of a Defect Free and Macrovoid Free Asymmetric Hollow Fiber Membrane from Torlon® (a Polyamide-Imide Polymer)
• Crosslinkable Polyimide Asymmetric Hollow Fiber Membranes for Aggressive Natural Gas Feed Streams

### Polymer Processing and Rheology I
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Early Structure Development during Flow-Induced Crystallization of Bimodal Blends of Model Isotactic Polypropylenes
• *In Situ* Synchrotron Studies of Structure Development during Injection Molding of a Liquid Crystalline Polymer
• The Role of Flow-Enhanced Crystallization in the Dynamics of Fiber Spinning
• Predicting the Coupled Development of Flow Induced Nanostructure, Rheology, and Performance Properties of Polymer/Nanoparticle Composites
• Effect of Processing Parameters on Microstructure and Tensile Properties of poly(L-lactic acid) (PLLA) Using Micro-Injection Molding
• Influence of Residual Stresses on the Creep Rupture Performance of Polyethylene Pipes
• High-Speed Microstructuring of Polymer Films Driven by a Fluid Dynamical Instability

### Polymer Thermodynamics I
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Phase Behavior of Supramolecular Diblock Copolymers
• Stability of the Gyroid Phase in Diblock Copolymers at Strong Segregation
• Self Consistent Field (SCF) Calculations of Mixed Neutral and Charged Polymer Brushes
• Ordering in Block Copolymer Thin Films Induced by Compressible Solvents
• Thermodynamics of Non-Isothermal Polymer Flows: Experiment, Theory and Simulation
• Glass Transition Temperatures of Biopolymer - Carbon Dioxide Systems
• Salt Analysis of Polystyrene, Polydiene, and Polystyrene-Block-Polydiene Phase Behavior in Propane
• Structure and Thermodynamic Properties of Linear - Tri-Arm Polyolefin Blends Based on Novel Atomistic Monte Carlo Simulation Schemes
• Simulation of Mechanically-Assembled Monolayers Using Discontinuous Molecular Dynamics

### Polymer Thin Films and Interfaces I
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Elastic Moduli of Ultrathin Amorphous Polymer Films
• Characterization of the Shear Moduli of Polymer and Polymer/Solvent Systems Using a Thin-Film Coated Thickness-Shear Mode (TSM) Quartz Resonator
• Quantifying Nearly Isochoric Glass Formation and the Extent of Physical Aging toward Equilibrium in Confined Polymer Films
• Role of $CO_2$ in Surface Tg Reduction of Polymers
• Friction at the Interface of Immiscible Pbd/ Pdms Polymer Melts
• Internal Structure and Charge Compensation of Polyelectrolyte Multilayers
• Transient Surface Patterns during Adhesive Contacts:Coalescence and Spreading of Liquid and Polymer Films
• Glass Transition and Ion Transport in Hydrogen Bonded Thin Film Layer-by-Layer Assemblies

### PSA/TSA/LSA
***Hilton San Francisco, Powell***
• $CO_2$ Capture from Flue Gas Using a Modified Duplex Pressure-Swing Adsorption
• Adsorption Process for C4 Olefin/Paraffin Separation
• VPSA Plant for Co Separation from Syngas with CUCLl/Zeolite
• Technology Developments in PSA Ethanol Dehydration
• Simulation of a Short-Bed, High Frequency PSA Cycle for Oxygen Concentration from Air
• How Favorable Isotherm Is Favorable in Pressure Swing Adsorption?
• Layered Bed Pressure Swing Adsorption Cycle for the Atmosphere Revitalization System of the Nasa Crew Exploration Vehicle

### Self-Assembled Biomaterials
***Hilton San Francisco, Union Square 23***
• Understanding, Chirality, Phase Behavior and Ordering in Aqueous Suspensions of fd Virus
• Disassembly of Layer-by-Layer Films of Plasmid DNA and Reducible Tat Polypeptide
• Towards an in Vitro Model of Anti-Therapeutic Resistance: Drug Efflux Pump Supported Membranes Tethered on Silica Microstructures
• Self-Assembled Protein Polymers for the Development of Nanostructured Biomaterials
• The Kinetic Evolution of Mixtures of Anionic and Cationic Lipid Vesicles
• Interactions between Fibrinogen and Peg Polymers in Aqueous Solution
• Microscopic Structure and Rheology of Salt-Responsive Hydrogels

### Special Session in Memory of Professor Koichiro Nakanishi
***Hilton San Francisco, Continental 4***
• Measurements and Predictions of Hydrate-Containing Phase Equilibria for CO2, Methane and Ethane in the Presence of NaCl
• From the Van der Waals to a Universal Group Contribution Equation of State
• Simulation Studies of Pattern Recognition: What's the Problem?
• Measurements of Partial Derivative Properties — Diffusion Coefficients and Spinodal
• Liquid Structures and Thermodynamic Properties of Lennard-Jones Mixtures

### Symposium Honoring CACHE Award Recipients (Invited Papers)
***Hilton San Francisco, Grand Ballroom A***
• Introduction of James M. Douglas, Winner of the 2006 ASEE / CACHE Award for Excellence in Computing in Chemical Engineering Education
• How Conceptual Design of Chemical Processes Can Be a Computer Aid
• A Module-Development Community to Advance Molecular Simulation in Chemical Engineering Education
• A Proposal for Diabetes Teaching Modules for the Undergraduate Chemical Engineering Curriculum
• Highlights of FOMMS 2006
• Highlights and Perspectives from the CACHE Conference on Chemical Process Control VII
• Enhancing Problem Solving in Excel and Matlab with Polymath 6.1

### Thermodynamic and Transport Properties in near and Supercritical Fluids
***Hilton San Francisco, Union Square 5 & 6***
• Permeability of $CO_2$ in Amorphous and Crystalline Teflon Membranes
• Quantification of the Interaction Energy between $Co_2$ and $Co_2$-Philes Using in Situ High-Pressure Goniometry and Tensiometry
• Crystallization and Gelation of Poly(4-Methyl-1-Pentene) in *n*-Pentane and in *n*-Pentane + Carbon Dioxide at High Pressures
• Group Contribution Estimation of Salt and Pc-Salt Parameters
• Structure-Based Generalizations of EOS Interaction Parameters for Predicting Vapor-Liquid Equilibria of Asymmetric Mixtures
• Correlation and Prediction of Transport Properties in near-Critical and Supercritical Fluids Using the Speadmd Model
• Probes of Supercritical $Co_2$ by Deflection of Multiple Beamlets

### Thermodynamic Properties and Phase Behavior III
***Hilton San Francisco, Union Square 19 & 20***
• Modeling of Electrolyte Systems with an Equation of State and Comparison with Molecular Simulations
• Vapor-Liquid Equilibrium of a Ternary System Containing Dimethyl Ether (DME) and Light Hydrocarbons
• Thermodynamic Validation of Asphaltene Phase Transition Phenomenon Using High Pressure NIR Cell
• Accurate Characterization of Intramolecular Contributions to the Thermodynamic Perturbation Terms

of Chain Fluids
• Liquid–Liquid Equilibrium Measurements for the Sulfur-Iodine Thermochemical Cycle: the Iodine-Water System
• Delivery of Fluorinated Prodrugs Using Perfluorooctyl Bromide as the Vehicle: Partition Coefficient Measurements and Membrane Fluidity Studies
• Experimental Densities of Benzothiophene, and Carbon Dioxide + Benzothiophene Binary Mixtures from 313 to 363 K up to 22 Mpa
• Using the Solvation Model to Predict the Salt Effect on Vapor-Liquid Equilibrium

**Thermophysical Properties of Biological Systems I**
***Hilton San Francisco, Union Square 1 & 2***
• A Computer Simulation and Theoretical Study of Hybridization in Model DNA Microarrays
• Monte Carlo Simulations of the Thermal Denaturation Transition of Model DNA Chains in Solution
• Unraveling the Behavior of DNA through Multiscale Modeling
• An Integrated Thermodynamical Approach to Predict the Melting Temperature and Stability of an Oligonucleotide Duplex in Solution and on Surface
• Role of Secondary Structure in Polymer Translocation through a Protein Nanopore: a Langevin Dynamics Study
• DNA Structure within a Virus Particle
• Molecular Dynamics Simulations of Viral Capsid Self-Assembly
• Structure and Osmotic Properties of DNA in Lambda Bacteriophages

**Transport and Reaction in Heterogeneous and Porous Systems**
***Hilton San Francisco, Franciscan A***
• Inertial Effects on Dispersion in Porous Media
• Models and Experiments on the Preparation of Silicon Carbide Microporous Membranes
• Development and Application of Modeling Tools for Mass Transport and Catalytic Reaction in Nanostructured Membranes
• A Novel Experimental Method to Identify Reaction Region in Reactive Viscous Fingering
• Optimization of Microfluidic Biofuel Cells Using Transport Principles
• Wormholing in Radial Flow
• Simulation of Random Sphere Packings Using an Evolutionary Optimization Method

**Transport in Nanoporous Materials**
***Hilton San Francisco, Sutter***
• Development of Fickian Diffusion Model for Mixtures in Nanoporous Adsorbents
• Molecular Simulation of Self- and Transport Diffusion of Mixtures in Metal-Organic Frameworks
• Modeling Gas Permeation in Nanopores
• New Silicoaluminophosphate and Titanosilicate Nanoporous Sorbents for Gas Phase Separations
• Characterization of Multicomponent Counter-Diffusion in Silicalite: Application to C6 Isomers in Liquid Phase
• Particle Impregnated Membranes for Bioseparations
• Mesoporous Ceramic Membranes for Non-Aqueous Separations: Surface Modification and Solvent Permeability

**Tuesday Workshop: What a ChE Educator Needs to Know about Bio**
***Hilton San Francisco, Imperial B***

**TUESDAY, 14 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**(22b) Nanotechnology and Nanobiotechnology for Sensors II**
***Hilton San Francisco, Plaza B***
• Immunoassay Sensors for Pathogen Detection Based on AC Dielectrophoresis and Self-Assembly of Carbon Nanotubes
• Temperature Controllable Stabilization/Surface Shielding of Gold Nano-Particles by Mononucleotides and Its Application in Synthesis of DNA-Gold Conjugates
• Characterization of Tethered Lipid Bilayers in Microfluidic Channels on Gold Surfaces
• Development of Affordable Bioelectronic Interfaces Using Medically Relevant Soluble Enzymes
• Single Molecule Measurements of Non-Exponential DNA Hybridization Kinetics
• Development of Novel Clinical Diagnostic Tools Using Zinc Selenide Quantum Dots as Fluorescent Labels
• Mass Transport in Analysis of Polynucleotides by Localized Surface Plasmon Resonance in Gold Nanoparticles on Optical Fibers

**(22b) Symposium on the 65th Birthday of Prof. Clark Colton Part III**
***Hilton San Francisco, Continental 5***
• Novel Charged Ultrafiltration Membranes for Protein Separations
• Immuno-Colton-Ization
• Vascular Cell Responses to Pressure
• Role of Ion Channels in Shear Stress Sensing in Vascular Endothelium
• A New Paradigm for Low Fouling Synthetic Membranes: Balancing Electrostatics
• Peptide Aggregation and Neurodegenerative Disease

**Advances in Biomaterials**
***Hilton San Francisco, Continental 4***
• Novel Biodegradable Amphiphilic Nanoadjuvants with Immunomodulatory Capabilities
• Synthesis and Characterization of Novel Functional Biodegradable Copolymer Composed of Ricinoleic Acid and L-Lactic Acid
• Preparation of Thermo-Responsive Polymer Gels Immobilizing Core-Shell Type Bioconjugates
• Poly(Diol Citrate) Nanocomposites with Enhanced Mechanical Properties
• Synthesis of Polylactide-Grafted Dextrans and Their Application as Biodegradable Biomedical Materials
• Swelling and Degradation Characteristics of Novel Biodegradable *in Situ* Crosslinkable Poly(Lactide-Ethylene Oxide-Fumarate) Terpolymer Networks
• Biomolecule-Responsive Behavior of Smart Gels Having Biomolecular Complexes as Reversible Cross-Links

**Advances in Distillation Modeling and Processes I**
***Hilton San Francisco, Mason***
• Analysis of Absorption with Nonequilibrium Complex, Reversible Chemical Reaction
• Solving Problems in Binary Batch Distillation on the Computer Using Mathcad® - Part 2
• Technological Study of $CO_2$ Capture Process with Mea
• A Principle of Corresponding States for Packed Column Pressure Drops
• A Rate-Based Model Approach to the Separation of Twelve-Component Hydrocarbons Mixture
• Using Distillation Column Profile Maps to Identify Suitable Thermodynamic Model for Complex Systems
• Minimum Energy for the Four-Product Kaibel Distillation Column
• Distillation Modeling the Cape Open Way
• Modeling and Optimization of Essential Oil Fractionation and Rectification Processes

**Advances in Protein Engineering (II)**
***Hilton San Francisco, Continental 7***
• Adapting Proteins to Accommodate Unnatural Amino Acids
• High Affinity FN3 Domains Using Loop Length Diversity and Population Maturation
• A Peptide Inhibitor Reveals a New Conformation of Transglutaminase 2
• Directed Evolution of the Luxr Transcription Factor for Applications in Synthetic Biology
• Engineering of a Carbazole Denitrogenation Pathway through Directed Evolution
• A Optimized Chimeric Estrogen-Sensor Protein: Applications in Drug Discovery and Biosensing
• Engineering of Blue Fluorescent Protein by Coupling Computational Design and Combinatorial Screening

**Advances in Proteomics: New Technologies I**
***Hilton San Francisco, Yosemite A***
• Characterization of Hep-G2 Conditioned Medium for Enhanced Mesoderm Differentiation of Es Cells: Application to Skeletal Tissue Engineering
• De Novo Peptide Identification Via Mixed-Integer Linear Optimization and Tandem Mass Spectrometry
• Dynamic Quantitative Analysis of the Nucleolar Proteome Using an Isobaric Mass Tagging Approach
• Enhancing Shotgun Proteomics Data Analysis with Bioinformatics Tools: Application to Cyanobacterial Proteomics
• Novel Selective Fluorescent Gel Stains for Improved Detection of Phosphoproteins
• Optimization of Chip-Based Infusion Nanoelectrospray Tandem Mass Spectrometry for the Rapid Analysis of Complex Proteomes

**Biomaterials for Tissue Engineering I**
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Novel Polyurethane Porous Foam Scaffolds for Bone Tissue Engineering Applications
• Peg-Based Hydrogels as Vocal Fold Regeneration Matrices
• Informatics and Data Mining of Combinatorial Datasets for Cell-Material Interactions
• Inverted Colloidal Crystals with Highly Controllable Structural Properties as Bone Tissue Engineering Scaffolds
• Nanoporous Multilayer Surfaces for the Design of Tissue Engineered Corneal Epithelium
• Growing Tissue-like Constructs with $Hep_3b/Hepg_2$ Liver Cells on PHBV Microsphere Scaffold
• Endothelialization of PLG Microsphere-Based Scaffolds for Bone Repair: Growth and Gene Regulation of Human Endothelial Cells

**Biomems and Biosensing**
***Hilton San Francisco, Continental 9***
• Numerical Optimization of a Biochemical Sensor Array
• Immunophenotyping of Leukocytes on Antibody Microarrays
• Effect of Eukaryotic Signaling Molecule Spatio-Temporal Gradients on Pathogenic *E. Coli* Colonization and Infection
• *Ex Vivo* Expansion and Differentiation of Haematopoietic Stem Cells (BSCS) Using on-Line Monitoring and Design of Experiments (Doe): Case Study of Erythropoiesis of Cord Blood Stem Cells
• Facile *in Situ* Protein Assembly Onto Patterned Electrodes and into Microfluidic Channels through Enzymatic Activation of Genetically Engineered Pro-Tags
• Quantitative and Simultaneous Detection of Four Foodborne Bacterial Pathogens with a Multi-Channel Spr Sensor in Complex Media
• Effect of Temperature, Analyte Concentration and Cell Growth Phase on the Luminescence of Pseudomonas Putida Tva8 Induced by Trichloroethylene

**Biomolecules at Interfaces IV - from Bacterial Adhesion to the Influence of an Electrical Potential**
***Hilton San Francisco, Union Square 22***
• Protein Film Voltammetry: from New Excitation Waveforms to Novel Signal Processing Techniques
• Single Molecule Force Measurements: New Insight into Biomolecules
• Colloidal Bridging Forces from Multiple Tethered Ligand-Receptor Bonds

• Bacterial Fouling Characteristics of the Surfaces of Poly (Ethylene Glycol), Dextran and Zwitterionic-Based Material
• Modeling Protein Adsorption with Electrochemical Impedance Spectroscopy
• Impedance Biosensors through Direct Protein Immobilization Onto Au
• Amyloid Assemblage-Lipid Interactions
• Continuous Polypeptide Adsorption under an Applied Electric Potential
• Dynamic Interactions of Live Group B Streptococci with Soluble and Adsorbed Fibronectin
• Insulin Fibrillation Kinetics at Interfaces

### Case Studies in Product Design - II
***Hilton San Francisco, California Room***
• Process Synthesis Applied to the Food Industry
• Design of a Microfluidic Chip for High-Throughput Screening of Kinase Inhibitors
• Marine Biofouling Protection: Design of Controlled Release Antifouling Paints
• Designing a Non-Soap Personal Washing Bar
• The Role of Solubility Modeling and Crystallisation in the Design of Active Pharmaceutical Ingredients
• Design of Liquid Enzyme Products with Built-in Detergent Stabilization System

### CAST Plenary Session
***Hilton San Francisco, Grand Ballroom A***
• Report by CAST Chair
• Dynamic Oil and Gas Production Systems Optimization Via Explicit Reservoir Multiphase Flow Simulation
• Electromechanically-Driven Complex Morphological Evolution of Void Surfaces in Metallic Thin Films
• Integrated Process Networks: Nonlinear Control System Design for Optimality and Dynamic Performance
• Process and Molecular Design: a Simultaneous Approach
• Smart Plants and Smart People

### Catalysis with Mesoporous and Microporous Materials II
***Hilton San Francisco, Franciscan C***
• Dimethyl Ether Carbonylation to Methyl Acetate on Acidic Zeolites
• ETS-10 and Vanadium-Doped ETS-10 Photocatalysts for VOC Decomposition Using Visible Light
• Photocatalytic Degradation of Organic Contaminants Using Multifunctional Titanosilicate ETS-10
• Preparation of Cu/ZnO and Cu/ZnO/$Al_2O_3$ Methanol Catalysts by Gas-Phase Loading of Mesoporous Silica: Towards Superior Catalytic Activity by Molecular Control of Their Microstructure
• The Synthesis of SWNT Supported Co Catalyst and Comparison with MCM-41 Supported Co
• The Optimal Network of Macro-/Mesopores in a Catalyst Pellet
• Statistical Design and Modeling of the Process of Methane Partial Oxidation Using V-MCM-41 Catalysts and the Prediction of the Formaldehyde Production

### Colloidal Dispersions II - Stability & Dispersion
***Hilton San Francisco, Union Square 25***
• Modeling Nanocolloidal Van der Waals Forces
• Mechanism of Enhanced Aggregation of Alginate-Coated Hematite Nanoparticles in the Presence of Calcium, Strontium, and Barium Cations
• Dispersion Characteristics of Oxide Nano-Particles in Sol-Gel Coatings
• Connecting the Depletion Flocculation and Interfacial Wetting Behaviors of Polymer-Grafted Nanoparticles in Polymer Solutions and Melts
• Stability and Aggregation of Dipalmitoylphosphatidylcholine (DPPC) Vesicles and DPPC-Fibrinogen Interactions
• Non-Spherical Armored Bubbles: Response to Mechanical Stress and Surfactants
• The Influence of Low Methanol Concentrations in Surfactant Solutions on Hydrate Anti-Agglomeration

### Complex-Fluid and Bio-Fluid Dynamics II
***Hilton San Francisco, Union Square 15 & 16***
• A Multi-Scale 3-D Computational Model Predicts That Cell Deformation Influences the Shear Threshold Phenomenon
• Modeling Release of Nanoparticles from Mobile Microcapsules
• Hydrodynamic Interactions during AFM Imaging of Biological Cells: Can AFM Truly Resolve Lipid Membrane Position?
• Dynamics of Vesicles in Linear Flows
• Prediction of Rheological Properties of Structured Fluids in Homogeneous Shear Flows Based on a Realizable Model for the Orientation Dyad
• Platelet-Platelet Collisions and Brownian Motion of Platelets near a Surface
• Cellular Contact Area and Detachment in a Shear Flow
• Formation of Stable Wrinkles and Tips on Skalak-Type Membranes
• A Computational Approach to Soft-Tissue Fluid-Structure Interaction
• A New Dielectrophoretic Theory for Red Blood Cells: the Role of Internal and External Double Layers

### Composites II
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Exfoliated Nanocomposite Powders- a Route to Lower-Cost Fillers
• Gas Separation Using Bromine Modified 2,4-Dimethyl-1,6-Phenylene Oxide/Silica Nanocomposite Membranes
• Mechanical Properties of Nanocomposite Systems
• Benign Process for Generating Low Density and Microcellular Poly(Ether Sulfone) Nanocomposite Foam
• Nanocomposites of Polyurethane Elastomers
• Cyanate Ester/Trisilanolphenyl-POSS Nanocomposites
• Micromechanics Simulations of the Viscoelastic Properties of Highly Filled Composites by Material Point Method

### Computational Studies of Self Assembly I
***Hilton San Francisco, Union Square 3 & 4***
• Atomistic and Coarse Grained Simulation of the Aggregation of Beta-Peptides in Solution
• Molecular Simulation of Amphiphilic Dendrimers
• The Pair of Potential of Mean Force for Helical Homopolypeptides
• Self-Assembly of Complex Polymeric Vesicles
• Multi-Scale Modeling of Self-Assembly in Surfactant Systems
• A Molecular-Thermodynamic Theory of Micellization of Mixtures of pH-Sensitive and Conventional Surfactants
• Phase Diagrams of Symmetric Diblock Copolymers Confined between Two Homogeneous Surfaces
• Effects of Polydispersity on the Stability of Aqueous Block Copolymer Assemblies
• Simulation Studies of the Stability of Phospholipid Bilayers in Clathrate Hydrates

### Crystallization of Pharmaceutical and Biological Molecules - I
***Hilton San Francisco, Lombard***
• Producing Small Crystals of a Pharmaceutical Compound by a Continuous Polymorph Transformation Process
• Rapid Expansion of Supercritical Solution with Solid Cosolvent (RESS-Sc) Process for Pharmaceutical Nanoparticles Formation
• Characterizing Intermolecular Interactions from Self-Diffusion Coefficients to Locate Conditions for Spherical Crystallization
• Concomitant Polymorphism in Industrial Precipitation Processes
• Phase Diagrams to Optimize Scale-up in Co-Crystal Systems
• High Throughput Nanoliter Screening and Morphological Control of Protein Crystals Via Precipitant Gradients

### Developments in Thermochemical and Electrolytic Routes to Hydrogen Production: Part IV
***Hilton San Francisco, Taylor***
• Platinum Group Metal Catalysts for Sulfur-Based Thermochemical Water Splitting Cycles
• Sulfuric Acid Decomposition with Heat and Mass Recovery Using a Direct Contact Exchanger
• Decomposition of Sulfuric Acid to Produce Sulfur Dioxide and Oxygen in Is Cycle
• A Corrosion Resistant Sulfuric Acid Decomposer for the Sulfur-Iodine Process
• Solar Configuration Study of Sulfuric Acid Thermal Decomposition in the S-I Thermochemical Hydrogen Production Process

### Fundamental of Fluidization II: in Honor of Prof. Bob Pfeffer on the Occasion of His 70th Birthday
***Hilton San Francisco, Franciscan D***
• Microparticle Flow in Liquid Medium: 3-D Velocity Measurements in Microchannels
• Effect of Solids Loading, Reynolds Number, and Particle Size Distribution on Velocity Fluctuations in Fluid-Particle Flows
• Enhanced Fluidization of Cohesive Particles by Surface Modification
• Functionalization of Ultrafine Particles by Atomic Layer Deposition in a Fluidized Bed Reactor
• Theoretical Studies of Nanoparticle Fluidizations
• The Effect of Drag Laws on the Prediction of Fluidized Bed Bubbling
• 3 Dimensional Numerical Simulation of Horizontal Rotating Fluidized Bed
• A Rotating Fluidized Bed in a Static Geometry: Experimental Proof of Concept

### Fundamental Research in Transport Processes II
***Hilton San Francisco, Union Square 21***
• Anomalous Heat Transfer in Granular Matter
• The Extraordinary Effects of an Energetic, Homogeneous Chemical Reaction on Internal Convective Heat Transfer in Tubular Flow
• Transport Properties of a Reacting Binary Fluid,from Non-Equilibrium Molecular Dynamics Simulations
• Optical Resonance Technique for Determination of Radial Concentration Distributions in Rapidly Evaporating Microdroplets
• Laser-Induced Luminescence Technique for the Simultaneous Measurement of Local Film Thickness and Temperature Distribution in Thin Wavy Liquid Films
• Fluid Dynamics and Heat Transfer of Viscous Falling Films
• A New Heat Balance for Flow Boiling

### Fundamentals of Environmental Catalysis II
***Hilton San Francisco, Franciscan B***
• Modeling $NO_x$ Storage on Pt-Ba/Alumina Catalysts
• Various Roles of Water in the Pt-Ba/Alumina Lean $NO_x$ Trap Catalysts
• Mechanistic Investigation of NSR (Nitrogen Oxide Storage and Reduction) Catalysts
• Lean $NO_x$ Trap Pt-Ba/$Al_2O_3$ Model Catalyst: Stability and Reactivity of Barium Species under Different Purging Conditions
• Product Speciation during Regeneration of Lean $NO_x$ Traps
• Peculiar Changes in Pt Accessibility and Morphology for Pt/BaO-$Al_2O_3$ Lean $NO_x$ Trap Catalysts with Different Sulfation Levels
• Modeling and Experimental Tap Studies on the Kinetics of $NO_x$ Storage and Reduction over Pt/Alumina and Pt/Ba/Alumina Catalysts

### Fundamentals of Interfacial Phenomena II
***Hilton San Francisco, Union Square 13***
• Spontaneous Droplet Breakup in Constricted Capillary Channels
• Electroosmotic Mixing inside Polyacrylamide Gels Via Immobilized Silica Nanoparticles
• Nanotribological Properties of Gas-Phase Lubricants between Silicon Nano-Asperity Contacts
• Exact Solutions for the Adsorption of Dimer Molecules Onto Finite Width Lattices
• Electrochemical Instability at the Liquid/Liquid Interface and Micro-Emulsions Formation
• Fundamentals of Bubble Transport in an Ultrasonically Assisted Separation Process
• Capillary Waves at the Liquid-Vapor Interface and the Surface

### Gene Therapy and Delivery (I)
***Hilton San Francisco, Continental 8***
• Relationships between Molecular Properties of Polymer-Oligonucleotide Complexes and Cellular Antisense Activity
• Engineering Adeno-Associated Viral Vectors with Novel Cell Tropisms
• Engineering Cell Lines for the Production of Highly Replication Defective Herpes Simplex Virus Type 1 Vectors
• Flow-Enhanced Measurement of Virus Infectivity
• Linear-Dendritic Hybrid Polymers for Targeted Gene Delivery to Antigen-Presenting Cells *in Vivo*
• Controllable Concentration Gradients by Spatially Patterned Gene Delivery
• Rapid Modification of Retrovirus Surfaces for Targeted Gene Delivery

### Hydrogen Storage
***Hilton San Francisco, Union Square 14***
• First Principles Investigation of Adsorption and Dissociation of Hydrogen on the Mg2SiB Surface
• Molecular Modeling to Improve Hydrogen Adsorption in Metal-Organic Frameworks
• Dopant and Vacancy Effects on Hydrogen Adsorption/Desorption by Aluminum-Based Complex Hydrides
• Hydrogen Absorption/Desorption Study over LI-B-*n*-H Quaternary System
• Reaction Pathways in the Gas/Solid Hydrolysis of Chemical Hydrides as a Novel Approach to Hydrogen Storage and Generation
• The Role of Carbon in the Hydrogen Storage Kinetics of Lithium Metal Hydrides
• Prediction of Hydrogen Hydrates Equilibria under an Organic Compound
• The Use of Certain Promoters to Store Hydrogen in Low-Pressure Clathrate Hydrates

### In Silico Systems Biology II
***Hilton San Francisco, Imperial B***
• *In Silico* Bacterial Cells: from Generalized Coarse-Grained to Genome-Specific Modular Models
• Bifurcation Analysis of Stochastic Gene Networks
• Novel Framework for Identifying Objective Functions of Biological Systems
• Modeling Amino Acid Metabolism in Mammalian Cells - Towards the Development of a Model Library
• Cell-Cell Crosstalk Potentiates Cell Patterning during Development
• Regulation of the SH2 Domain-Containing Protein-Tyrosine Phosphatase SHP2 in Receptor Signaling: Kinetic Model and Structure-Based Analysis
• Molecular Signatures That Differentiate Cancer Subtype and Predict Clinical Outcome

### Introducing Chemical Engineering to K-12 through Experimentation and Course Integration II
***Hilton San Francisco, Van Ness***
• Process Technology Institutes and Workshops for K-12 Educators and Students
• Tennessee Technological University Math and Science Partnership
• Elementary Education Majors Learn How to Teach Science and Engineering from an Engineer
• Experiments in Science and Engineering: a Workshop for High School Science Teachers
• Ret Site: Inspiring Educators in Rural America through Research
• Course Module Development Using Nsf-Ret Site Program
• A Program for Introducing Engineering Concepts into High Schools and Middle Schools

### Invited: in Honor of Massimo Morbidelli, Wilhelm Award Recipient I
***Hilton San Francisco, Imperial A***
• Polymer Product Properties - Polymerization Leaves Distributions Everywhere
• Chemical Reaction Engineering for Economic Growth and Sustainable Development
• What Generates Transversal Hot Zones in Packed Bed Reactors
• Micro-Structured Reactors for Catalytic Processes
• Catalysis and Reactor Engineering with Carbon Dioxide-Expanded Liquids

### Membranes for Bioseparations II
***Hilton San Francisco, Continental 2***
• Separation of Macromolecules by Dynamic Ultrafiltration
• Further Study of the Effect of Electrostatic Properties in Binary Protein Ultrafiltration
• Membrane Cascades for Downstream Processing
• Ultrafiltration Characteristics of Plasmid DNA
• Techniques for Ultrafiltration Membrane Scale-up and Scale down
• Selective Separation of HIV-Tat Protein Using Functionalized Stacked Microfiltration Membranes: Enhancement of Flux and Recovery of Protein
• Evaluation of Affinity Membrane Adsorbers for Antibody Purification

### Mixed Matrix Membranes
***Hilton San Francisco, Yosemite B***
• Dendrimer-Ceramic Composite Membranes for Challenging Separations
• The Importance of Dope Stability in Mixed Matrix Hollow Fiber Membrane Formation
• Permeability Enhancement in Nanoparticle Filled Polymeric Membranes
• A Novel Ion Exchange Treatment of Zeolite for the Application of Mixed Matrix Membranes in Natural and Hydrocarbon Separation
• Bottom up Synthesis of Composite Membranes
• Facilitated Transport of Thiophenes through $Ag_2O$-Filled P D M S Membranes

### Modeling of Inorganic Materials Synthesis and Properties
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Modeling the Synthesis of Periodic Mesoporous Silicas
• Atomistic Simulation of the Formation of Nanoporous Silica Films Via Chemical Vapor Deposition
• Modeling the Formation of Geopolymers
• Growth, Structure, and Fractal Scaling in Silica Gels Produced by Polymerization of Aqueous Silicic Acid
• Molecular Dynamics Simulation Study on the Morphological Control of Alpha-Al2O3 Nanoparticles
• Strain Energy Minimum and Vibrational Properties of Single-Walled Aluminosilicate Nanotubes
• Multiscale Modeling of Relaxor Ferroelectrics

### Modeling and Control for Diabetes Applications
***Hilton San Francisco, Continental 3***
• Prandial Insulin Dosing Using Run-to-Run Control: Application of Clinical Data and Medical Expertise to Define a Suitable Performance Metric
• Optimal Control of Diabetes Mellitus under Time Dependent Uncertainties
• Model Based Predictive Control of Blood Glucose Concentration in Type-I Diabetic Patients
• Dynamic Modeling and Model-Based Control of Exercise Response in Type 1 Diabetic Patients
• Linear and Recursive Models for Prediction of Blood Glucose Concentration
• An Experimental Evaluation of Pca Monitoring Strategies for Type 1 Diabetes Subjects

### Molecular Simulation of Adsorption I
***Hilton San Francisco, Sutter***
• Computer Simulation of Adsorption in Templated Molecular Recognition Materials
• Adsorption from Dilute Liquid Solutions: Molecular Dynamics Simulations Using the Mean Force Method
• Studies of a Lattice Model of Water Confined in a Slit Pore
• Water Condensation in Hydrophobic Zeolitic Nanopores
• Density Functional Theory Model of Adsorption on Amorphous and Microporous Silica Materials
• Molecular Simulation of Adsorption in Polycrystalline Nanoporous Materials
• GCMC Simulations of Adsorption of Argon in Slit Pores with Defected Walls

### Nanoparticle Synthesis and Stabilization
***Hilton San Francisco, Continental 1***
• Effect of Surfactants on Nanoparticle Surface Chemistry
• Hemispherical Polystyrene/Clay Nanocomposite Particle Formation in a Miniemulsion Polymerization
• Droplet and Particle Formation in the Electrohydrodynamic Atomization Process
• Nanoparticles for Hydrophilic and Antimicrobial Surface Coatings
• Ag and Au Monometallic and Bimetallic Colloids: Morphogenesis in Amphiphilic Block Copolymer Solutions
• Kinetic Study of Ag2s Fluorescent Nanoparticles Synthesis
• Aggregates Size/Structure and Rheological Properties of Nano-Sized Goethite Aqueous Suspension

### National Science Foundation Workshop I
***Hilton San Francisco, Plaza A***
• NSF Overview
• Shared Cyber Infrastructure and Complex Systems
• NSF Engineering Emerging Frontiers Research Initiative
• Question & Answer Session I
• NSF Engineering Research Centers Activities
• NSF Engineering Education Activities
• Small Business Innovation Research Partnership Opportunities
• Discussion by Interagency Representatives
• Question & Answer Session and Announcements

### Non-Newtonian Flows
***Hilton San Francisco, Union Square 17 & 18***
• Understanding the Viscoelastic Properties of Extruded Polypropylene Wood Plastic Composites
• Computational Studies of the Motion of a Nematic LCP in a Simple Shear Device
• Structure and Rheology of Shear-Banding Wormlike Micellar Solutions
• Rheo-Optics of Equilibrium Polymer Solutions: Wormlike Micelles in Planar Elongation
• Extentional Rheometry on a Chip: Flows of Dilute Polymer Solutions in Microfluidic Contractions
• Low-Dimensional Models for Exact Coherent Structures in Viscoelastic Shear Flows
• Viscoelastic Nonlinear Traveling Waves and Drag Reduction in Plane Poiseuille Flow
• Effect of Flexibility on the Shear-Induced Migration of Short Polymers in Parabolic Channel Flow
• Elastic Instabilities of Polymeric Solutions in Cross-Channel Flow

• Dynamics of Polymeric Solutions in Prototypical Processing Geometries: a Multiscale Simulation Approach
• Comprehensive Modeling of Nonisothermal Polymer Jets in Melt Electrospinning

**Novel Adsorbent Materials and Structures I**
***Hilton San Francisco, Powell***
• Cu-BTC: a Shape Selective Mom Material for the Adsorptive Separation of *n*- and Iso-Alkanes
• Towards the Rational Design of Metal-Organic Frameworks: Using Molecular Simulations to Understand Adsorption Phenomena in MOFs
• Design, Synthesis, and Applications of Reversible Oxygen Chemisorbents
• Microfibrous Entrapment of Zeolites for High Duty Cycle Oxygen Enrichment from Air
• Porous Iron Oxyhydroxide Having Dual Adsorption Site for Efficient Removal of Anions in Wastewater
• Adsorption Properties of Mesoporous Alumino and Titanosilicates of MCM-41 Type
• Effect of Pore Size Distribution and Surface Area of Activated Carbon Fabrics for the Liquid Phase Adsorption of Chemical Warfare Agent Simulants

**Novel Computational and Experimental Methods in Mixing**
***Hilton San Francisco, Union Square 23***
• Millisecond Mixing of Two Liquid Sheets in a Jet Nozzle
• Experimental and CFD Studies on Micromixing in a Multi-Inlet Vortex Mixer (Mivm)
• Flow Characteristics of a Sawtooth Impeller
• Large Eddy Simulation of an Inline Rotor-Stator Mixer and Comparison with High Resolution Piv Measurements
• Break up of Nanoparticle Clusters Using an in-Line Rotor-Stator- Validated CFD Result
• Design of a Low Shear Hydrofoil through the Use of Computational Fluid Dynamics and Multi-Objective Design Optimization
• Effect of Paddle Position and Tablet Location on the Hydrodynamics of USP Dissolution Testing Apparatus 2

**Polymer Processing and Rheology II**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Effects of Additives on Rheological Properties, Atomization, Drying Duration, and Coating Strength of Polyethylene Oxide Aqueous Solution
• Correlating Branch Content Information from Rheological Studies and Small Angle Neutron Scattering
• Transient Recovery after Extentional Flow of Elastomeric Random Copolymers
• The Effect of Rheological Properties on Film-Casting Performance
• Polymer Dynamics and Rheology in Designing and Understanding Polymeric Biomaterials for Tissue Engineering Applications
• A Semi-Empirical Model for the Prediction of the Rheological Behavior of Polystyrene Samples over a Wide Range of Molecular Weights
• A Molecular Dynamics Study of the Stress-Optical Behavior of a Linear Short-Chain Polyethylene Melt under Shear
• Modeling Polymer Melts Containing Short and Long Fibers: Part I Transient Rheology

**Polymer Thermodynamics II**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Influence of Long Molecule Architecture on the Morphology and Properties of Oriented Polyethylene Films
• Manipulating Structures of Block Copolymers with Functionalized Layered Silicates
• Solution Behavior of Stereoregular Polyelectrolyte
• A Comparison of Direct and Indirect Methods for Calculation of Polymer Solubility Parameters from Molecular Simulations
• Synthesis of Amphiphilic Copolymers and Assessment of Their Critical Aggregation Concentrations Via Fluorescence Techniques: Styrene/Acrylic Acid Diblock, Random and Gradient Copolymers
• The Importance of Quenched Randomness of Stereochemical Sequences in Atactic Vinyl Polymers and Implications for Coarse-Graining
• Kinetics of Pressure-Induced Phase Separation in Polystyrene-Acetone Solutions at High Pressures. Binodal and Spinodal Envelopes
• Molecular Simulation of the Influence of Nanoparticles on the Bicontinuous Phases of Diblock Copolymer Melts

**Polymer Thin Films and Interfaces II**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Photoalignment Behavior of Liquid Crystals on Coumarin-Containing Polymer Films
• Determination of Interfacial Properties of Polydimethylsiloxane-Water Systems Using Molecular Dynamics Simulations
• Density Functional Theory for Polyelectrolyte Brushes
• Integrating Plasma Surface Initiation with "Living" Nitroxide-Mediated Polymerization: Novel Approach to Graft Polymerization
• New Photodefinable Dielectric Polymer Thin Film Materials for Microelectronics and Optoelectronics Based on Novel Hexafluoralcohol Substituted Monomers
• Correlation of Polymeric Surfactant Film Surface Characteristics to Nanotribological Performance
• Nanoscale Relaxation, Transition and Structure Properties of Organic Thin Film Electronic Materials

**Polymeric and Other Organic Materials as Membranes for Gas and Vapor Separation**
***Hilton San Francisco, Yosemite C***
• Analysis of the Solubility of Gases in Mixed Matrix Membranes through the NELF Model
• Mixture Permeability, Solubility, and Diffusivity in Vapor Selective Polymers
• Hydrogen Sulfide and Carbon Dioxide Removal with Facilitated Transport Membranes
• Mixed Gas Selectivities and Permeabilities for Carbon Dioxide/Methane Separation Using Facilitated Transport in Room Temperature Ionic Liquid Membranes
• Langmuir-Blodgett Films with Fluorinated Surfactants Bilayers on Polymer Supports as Membrane for Gas Separations

**Reaction Path Analysis I**
***Hilton San Francisco, Franciscan A***
• In-Situ Infrared Study of Catalytic Ignition of Methane on $Rh/Al_2O_3$
• On-Line Spectroscopic Studies and Kinetic Measurements of Liquid-Phase Heterogeneous Catalytic Systems
• Elucidating the Reaction Pathway for Water-Enhanced Cycloaddition
• Mechanistic Studies of Olefin Epoxidation by Hydrogen Peroxide Catalyzed by Iron Porphyrins
• Ab Initio Reaction Path Analysis of the Initial Hydrogen Abstraction from Organic Acids by Hydroxyl Radicals
• Kinetic Study of Acrylate Polymerization at High Temperature
• A First-Principles Analysis of the Synthesis of Organic/Inorganic Hybrid Nanoscale Systems: Epoxy Amine Addition for Polysilsesquioxanes
• A Density Functional Theory Study of Reaction of $H_2$ and $O_2$ to Form $H_2O_2$ on Gas-Phase Au-Alloy Clusters

**Reactions in near and Supercritical Fluids I**
***Hilton San Francisco, Union Square 5 & 6***
• Solvent Effects in Ionic Liquid Production in Conventional and Dense-Phase $CO_2$ Systems
• Solvent-Free Synthesis of Poly (Phenylene Ether) (PPE) in Supercritical Carbon Dioxide
• Catalyst and Media Alternatives in the Oxidation of P-Xylene to Terephthalic Acid
• Supercritical Fluid Oxidation of Oleic Acid
• Solid Acid Catalyzed Esterification of Free Fatty Acids in Oil Using $CO_2$ Enhanced Media
• Density Functional Theory Study of Glyceraldehyde Hydrolysis in Supercritical Water

**Solid Liquid Interfaces**
***Hilton San Francisco, Union Square 24***
• Probing Nano-Domains in Single Bilayer Bio-Membranes Using Grazing Incidence X-Ray Diffraction
• Dynamic Wetting Behavior of Complex Liquids on Rough Surfaces
• Dynamics and Collapses of Colloidal Lattices at Oil - Water Interfaces
• Surfactant and Electric Field Strength Effects on Surface Tensions at Liquid/Liquid/Solid Interfaces
• Polarizable Contributions to the Surface Tension of Liquid Water
• Solid-Liquid Interfacial Energy of the Polymorphs of Paracetamol
• Molecular-Based Study of the Graphene/AqMOIueous Polyelectrolyte Interface toward the Understanding of PEM Formation

**Sustainability of Drinking WMOI ter Supply**
***Hilton San Francisco, Continental 6***
• The U. S. National Science Foundation's Cleaner Initiative
• Mapping Multiple Interactions: Social Relations and Nutrient Loading in Source Water
• Purification of Water Using Nanotubes
• Development of Hybrid Ultrafiltration Combined with Both Flocculation and Adsorption Treatments for Advanced Removal of Humic Substances
• Preparation of Porous Poly(Vinyl Butyral)-Tio2 Composite Hollow Fiber Membrane for Drinking Water Treatment
• Depth Filter Membranes of Biodegradable Polyesters
• Fouling Monitoring during Microfiltration of Surface Water by Filtration Resistance and Streaming Potential

**Thermodynamic Properties and Phase Behavior IV**
***Hilton San Francisco, Union Square 19 & 20***
• A Family of Entropy-Based Anomalies for a Water-like Fluid
• Advanced Fluid Property Measurement and Prediction for Oilfield Applications
• Phase Equilibria of Mixtures of Amines with Alcohols, Ketones and Nitriles
• Higher Order Virial Coefficients and Molecular Clustering of Polarizable Water Models
• A Statistical Mechanical Perspective on Linear Free Energy Relationships
• On the Use of Scaled Particle Theory to Determine a Broad Range of Hard-Sphere Fluid Properties with High Accuracy
• On the Determination of the Dipole Moments of Solutes from Multi-Component Systems: Experimental and Model Development
• Modeling Pharmaceutical Salt Solubility in Mixed Solvents with Enrtl-Sac

**Thermophysical Properties of Biological Systems II**
***Hilton San Francisco, Union Square 1 & 2***
• Heteropolymer Collapse Theory for Protein Folding in the Pressure-Temperature Plane
• Molecular Dynamics Study of Pressure Denaturation of Proteins
• Characterization of the Phase Behavior of Phospholipid Bilayers
• Using Molecular Simulation to Explore the Phase Behavior of a Simple Model Protein
• Role of Fluctuations in a Snug-Fit Mechanism of the Kcs K+ Channel Selectivity
• Mechanical Properties of Proteins: the Dynamic Energy Landscape
• Dynamical Motions of Lipids and a Finite Size

Effect of Bilayers
• Computational Investigation of Cold-, Heat-, and Pressure-Induced Protein Unfolding with an Explicit-Water Protein Model

**TUESDAY, 14 NOVEMBER 2006**
***3:15 PM - 5:45 PM***

**(22a) Carbon Nanotubes IV**
***Hilton San Francisco, Yosemite B***
• Electrostatically Modulating the Transport Properties of Carbon Nanotube Membranes
• Porous Hollow Carbon Nanotube Composite Cages
• Length Dependent Anisotropic Polarizability of Single Wall Carbon Nanotubes Measured Via the Electro-Optical Effect
• Metallized Single-Walled Carbon Nanotubes for Hydrogen Sensor Applications: a DFT Study
• Brownian Dynamics Simulations of Single-Wall Carbon Nanotube Separation by Type Using Dielectrophoresis
• Metals and Metal Oxides Nanoparticles Decorated SWNT Networks

**(22b) Nanotechnology and Nanobiotechnology for Sensors III**
***Hilton San Francisco, Plaza B***
• Detection of Viruses by Nanoscale Spm-Based AC Impedance Spectroscopy
• Nanoparticle Assemblies: Optical and Electrical Properties and Their Biomedical Sensing and Imaging Applications
• Evanescent Field Response to Patterned Features on a Planar Waveguide Biosensor
• Biocompatible, Fluorescence Enhancing Solvents for Sensitive Fluorophore Mediated Biosensor and Observation of Protein Conformation Change by Atomic Force Microscopy
• Immunosensing Arrays Based on Air-Stable Tethered Lipid Membrane Mimics and Ligand-Gated Ion Channels
• Electrochemical Platform for Impedimetric Immunosensors
• Synthesis and Ft-Irras Characterization of Ir-Active Bionanomaterials from Fourth Generation Polyamidoamine Dendrimer
• Electrochemically and Chemically Functionalized Single-Walled Carbon Nanotube Network for Gas Sensing

**(22b) Symposium on the 65th Birthday of Prof. Clark Colton Part IV**
***Hilton San Francisco, Continental 5***
• Hepatic Tissue Engineering
• Factors Influencing Monocyte Transport to Arterial Endothelium
• Transport in Biological Systems
• Making Molecules into Medicines: Engineering in Materials Properties
• Drug Absorption in the Upper Small Intestine and Its Implications in the Design of Oral Protein Delivery Carriers
• Technology Based Innovation in Healthcare: How Can We Do It Better?
• Chemical Engineering in Biology and Medicine: a Retrospective Perspective

**Advances in Biocatalysis**
***Hilton San Francisco, Continental 9***
• Biosynthesis of Novel Flavonoids through an Engineered Phenylpropanoid Pathway in *Saccharomyces Cerevisiae*
• Engineering of Synthetic Cytochrome P450s for Plant Estrogen Isoflavone Biosynthesis from *Escherichia Coli*
• P450 Biocatalysis in Two-Phase Aqueous-Organic Emulsions
• Heterologous Expression of Microbial Genes for Drug Metabolism in Gram Negative Bacteria
• Process and Enzyme Engineering of Aminotransferases for Improved Activity and Thermostability
• Alkyl Hydroperoxide Reductase & Water-Forming NADH Oxidase: Comparison and Application for Selective Oxidations
• Novel Biocatalyst for Simvastatin Synthesis

**Advances in Distillation Equipment & Applications**
***Hilton San Francisco, Mason***
• Effect of Pressure on Packed Column Distillation Efficiency
• Rectifier Design for Ethanol Plants
• Homogenous Azeotropic Pressure Swing Distillation – a Discussion of the Inverted and the Regular Batch-Process
• Continuous Three Phase Distillation: a Process for Separating Thermally Unstable Substances
• Design Considerations for High Liquid Rate Tray Applications
• An Analysis of Non-Equilibrium Thermodynamics to DDV Tray and the Determination of Its Performances
• Experimental Evaluation of Sulphur Dioxide Absorption in Water
• Microchannel Distillation of JP-8 Jet Fuel for Sulfur Content Reduction
• Total Reflux Batch Distillation with Dual Temperature Control

**Advances in Proteomics: New Technologies II**
***Hilton San Francisco, Yosemite A***
• Phosphopeptide Analysis Using a Planar Electrochromatography/ Thin-Layer Chromatography Separations Platform Coupled to Orthogonal Maldi-TOF Mass Spectrometry
• Pressurized Planar Electrochromatography: a New Tool for Proteomics?
• Proteomic Analysis of Immunogenic Proteins in Xenogeneic Heart Valve Bioscaffolds
• A Closer Look at E. Coli-Derived 6-Deoxyerythronolide B Biosynthesis
• Proteome Analysis of Pseudomonas Putida during Biodegradation of High Concentration of Benzoate:Activation of the Meta Pathway and Physiological Responses
• Validation of a Carrier Ampholine 2-D Electrophoresis System

**Advances in Therapeutic Bionanotechnology and Devices**
***Hilton San Francisco, Continental 4***
• Thermally Responsive Interpenetrating Polymer Network Nanoparticles
• Preparation of Temperature-Sensitive Liposomes for Delivery of Anticancer Drugs by Use of Thermosensitive Amphiphilic Block Copolymer
• Preparation of pH-Sensitive Core-Shell Type Polymeric Micelle from Poly(Peptide-B-Lactide) Diblock Copolymers as Biodegradable Biomedical Material
• Sequestration of Amitriptyline by Liposomes
• Development of a Regenerable Cell Culture Material System That Senses and Releases Dead Cells
• Novel *in-Situ* Hybrid Hydrogels of Hyaluronic Acid, Cellulose Derivatives, and Dextran to Prevent Peritoneal Adhesions

**Biocomposites**
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Layer-by-Layer Assembly of Novel Nanocomposites from Cellulose Nanocrystals
• Characterization of Biopolymer Composites Created Using Solid-State Shear Pulverization
• Fire Retardant Fatty Acid Based Vinyl Ester Resins
• Polymer-Nanotube-Enzyme Composites as Active Antifouling Films
• Electrodeposition of Lysozyme-Silver Antimicrobial Bionanocomposites Onto Stainless Steel Medical Instruments
• Adsorption and Desorption of Lysozyme on Thermosensitive Nano-Sized Magnetic Particles and Its Conformational Changes
• Composite Layered Scaffolds for the Regrowth of Heterogeneous Tissue

**Biomaterials for Tissue Engineering II**
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Oriented Collagen Films for Wound-Healing Applications
• Mechanically Stimulated Mesenchymal Stem Cells Form Tendon-like Tissue
• Mechanical Properties and Permeability of Collagen-Gag Scaffolds for Tissue Engineering: Cellular Solids Modeling and Experimental Results
• The Effects of Elastin on the Mechanical Properties of Collagen-Gag Membranes for Tissue Engineered Skin
• A Novel Formulation of Oxygen Carrying-Matrix Enhances Liver Specific Function of Cultured Hepatocytes
• Water and Solute Transport in a Tissue Engineered Pancreatic Substitute

**Biomolecules at Interfaces V - Controlling and Observing Interfacial Protein Behavior**
***Hilton San Francisco, Union Square 22***
• Modifying Antibody Immobilization Density with Mechanical Assembled Monolayers
• An *a Priori* Estimate of Oxygen Delivery at the Capillary and Skeletal Muscle Interface
• Interfacial Horseradish Peroxidase Spot Growth in the Aorta of Acute Hypertensive & Hypotensive Rats
• Temperature and pH Effects on Deposition Kinetics of Beta-Lactoglobulin
• Enzymatic Hydrolysis of Proteins in Bulk Solutions and at Liquid/Air, Liquid/Solid Interfaces: Effect of Surfactants
• Modeling Statherin Structure Binding to Hydroxyapatite [001] Crystal Surface
• Plasmid DNA Adhesion on Silica: Kinetics and Conformational Changes in Mono and Divalent Salts
• Kinetics of Unfolding of Adsorbed Beta Lactoglobulin on Silica Nanoparticle Surface
• Thermodynamic Characterization of Copper Biosorption Process by Pretreated a. Niger Biomass

**Bioprocess Modeling and Control**
***Hilton San Francisco, Continental 7***
• Systematic Development of Predictive Mathematical Models for Animal Cell Cultures
• Modeling and Control of a Rotating Disk Bioreactor
• Analysis of Culture Phases in Threonine-Limited Lysine Fermentation Using 2-Dimensional Electrophoresis
• A Comprehensive Kinetic Investigation of Enzymatic Hydrolysis of Cellulose
• Genome-Scale Analysis of Saccharomyces Cerevisiae Metabolism and Ethanol Production in Batch and Fed-Batch Culture
• Robust Global Stabilization of Continuous
• Bioreactors
• The Development of New Experimental Design Method for Processes with High Non-Linearity and Dimensionality

**Colloidal Dispersion III - Structure & Rheology**
***Hilton San Francisco, Union Square 25***
• The Effect of Nanoparticles on the Structure and Rheology of Kaolinite Suspensions
• Direct Quantification of Gel Structure and Suspension Dynamics in Biphasic Colloidal Mixtures
• Nanoparticle Stability and Structure in Polymer Melts
• The Effect of Free Surfactant and Grafted Surfactant Surface Coverage on the Rheology and Microstructure of Organoclay Dispersions
• Structure and Elasticity of Polymer-Nanoparticle Gels
• Connections between Rheology and Structure of Attractive Colloidal Systems
• Shear Induced Diffusivity of Spherical and Non-Spherical Particles

**Computational and Numerical Approaches to Particle Flow**
***Hilton San Francisco, Franciscan D***
• Stress Distribution in the Avalanching Flow of

Cohesive Granular Materials in a Rotating Vessel
• Feasibility of a Coupled Discrete-Time Immersed Boundary-Discrete Element Method for Numerical Simulation of Granular Multiphase Flow
• Analyses on the Particle Flow in a Bed with Lateral Gas Blasting
• Why Do Continuum Gas-Solids Flow Models Predict Core-Annulus Flow?
• Revisiting the Standard Drag Law for Bubbling, Gas-Fluidized Beds
• Insights in Secondary Gas Injection in a Bubbling Fluidized Bed Via Discrete Particle Simulations
• Modeling of Suspension Flows in Coating Dies

**Computational Studies of Self Assembly II**
***Hilton San Francisco, Union Square 3 & 4***
• Monte Carlo Simulations of Self-Assembly for Amphiphilic Nanoparticles
• Icosahedral Packing of Polymer-Tethered Nanospheres and Stabilization of the Gyroid Phase
• Searching for Ordered Dense Packings of Particle Systems
• A Monte Carlo Analysis of Crystallization Free Energy Barriers in Colloidal Systems with DNA-Mediated Interactions
• Self Assembly of Nanoparticle-Polymer-Nanoparticle Triblocks
• Geometric Model of Depletion Forces in Hard-Sphere Colloidal Dispersions Exposed to Various Surfaces
• Cosmomic: Extending Cosmo-RS to Self-Assembled Structures
• Self-Assembly in Ternary Systems Containing Symmetric Amphiphilic Chains and Hybrid Organic-Inorganic Precursors
• Computational Design of a Single-Chain Four-Helix Bundle Protein with a Non-Biological Ru(II)Polypyridyl-(Porphinato)Zn(II) Cofactor

**Crystallization of Pharmaceutical and Biological Molecules - II**
***Hilton San Francisco, Lombard***
• Microfluidic Platforms for Protein Crystallization Screening
• Protein Crystallization in Protein Condensation Diseases: Apoferritin Crystallization in Cataract Formation
• Prediction of Cryoprotectant Requirements for Flash Cooling of Protein Crystals
• Crystallization in Surfactant-Free Monodisperse Emulsions
• Change of Polymorphs of Guanosine-5'-Monophosphate Using Drowning-out Crystallization
• Preparation of Dextran Microsphere Using Supercritical Antisolvent Process

**Developments in Thermochemical and Electrolytic Routes to Hydrogen Production: Part V**
***Hilton San Francisco, Taylor***
• High Temperature Electrolysis for Hydrogen Production Using Tubular Electrolyte Cells Assembly Unit
• Status of the R&D Effort for the Cu-CL Cycle
• Hydrogen Production by Thermochemical Water-Splitting Is Process
• Simulation of Sulfur-Iodine Thermochemical Cycle Coupled to Nuclear Heat Transport System
• Dynamic Flow of Micro-Channels in a Ceramic Heat Exchanger
• Optimizing the Micro-Channels Features in a Ceramic Heat Exchanger for Sulfuric Acid Decomposition

**Emulsions and Foams**
***Hilton San Francisco, Union Square 24***
• Nucleation and Bubble Growth Dynamics in Polymer Foaming on Paper Board
• Role of Micelles in Ostwald Ripening and Solubilization
• Using NMR to Study Hydrodynamic Forces in the Coalescence of Emulsions
• A Novel Production Method for Lipid-Stabilized Monodisperse Ultrasound Contrast Agents
• Peptide Surfactants (Pepfactants®) for Switchable Control of Foam and Emulsion Stability
• Rupture of Draining Foam Films Due to Random Pressure Fluctuations
• Particle-Induced Drop Bridging in Pickering Emulsions

**Fuel Cell Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Experiences with S.O.F.C. and CO-Producing Hydrogen
• Composite Polybenzimidazole/Polyimide-Clay-$H_3po_4$ Membranes for Use in Fuel Cell Applications
• Minimum Energy Path of Hydrogen in a Pt (111) Cluster
• Fuel Cell Applications: Synthesis and Characterization of Microporous Titanium Silicates for Use in Composite Inorganic-Organic Polymer Electrolyte Membranes
• Structure of Pt/Ir/Iro2 tubes and Their Electrocatalytic Properties in Oxidation of Small Organic Molecules
• Sulfonated Poly(Arylene Ether Sulfone)-Inorganic Oxide Nanocomposite Membranes Containing Organic-Metallic Complexes
• Electrochemical Performances of Non-Perfluorinated Membrane-Electrode Assemblies for Dmfc Application
• Characterization of the Gas Phase Hydrolysis of Sodium Borohydride
• A Study of Integration Potentials in Various Reformer Strategies for Logistical Fuels Processing
• Integration of Multi-Scale Multi-Phenomena Simulations of Direct Methanol Fuel Cell Via Lattice Boltzmann Methods
• Optimal Synthesis of Hybrid Power Plant

**Fuel Cell Technology I**
***Hilton San Francisco, Van Ness***
• MRI Investigation of Water Distribution in an Operating PEM Fuel Cell
• Water Management by Materials Design and Engineering of the Membrane and Electrode Assemblies
• Utilization of Metal Phthalocyanines as Cathode Catalysts of Proton Exchange Membrane Fuel Cells
• Microfluidic Fuel Cells
• PEM Fuel Cell Current Control by Fuel Starvation

**Fundamental Research in Transport Processes III**
***Hilton San Francisco, Union Square 21***
• Transient Effects on Secondary Flow Behavior in Double Bifurcation Model
• Unsteady State Separation of Multicomponent Mixtures in a Thermogravitational Column
• Molecular and Thermal Diffusion Coefficients of Binary Hydrocarbon Mixtures
• Effects of Dual Porosity during the Consolidation of Fibrous Media
• Turbulence Flow Structure Effects on Turbulent Heat Transfer
• A New Theory to Explain Transport in Pulsed-Flow Bubble Columns: the Bjerknes Effect
• Compact Polymeric Hollow Fiber Heat Exchangers (PHFTEs): Multiscale Performance Studies and Modeling
• Natural Convective Heating in Food Materials in Cylinders

**Fundamentals of Environmental Catalysis III**
***Hilton San Francisco, Franciscan B***
• Lean $NO_x$ Trap Morphology Changes with Lean/Rich Cycling
• Novel Analytical System for Exhaust Emissions Control Catalysts
• On the Selective Catalytic Reduction of NO with Methane over Ag-Alumina Catalysts in the Presence of $SO_2$
• Decomposition of Nitric Oxide by Platinum Supported on Tin Oxide
• The Effect of Sulfur Dioxide on Hydrogen Promotion of the Hydrocarbon Selective Catalytic Reduction of Nitric Oxide under Lean Conditions over $Ag/Al_2O_3$
• Application of $V2O_5$ in NOx Reduction and Evaluation of Various Effects on Variation of Its Activity
• An Investigation of the Thermal Stability and Performance of Wet-Incipient WO3/V2o5/Tio2 Catalysts and a Comparison with Flame Aerosol Catalysts of Similar Composition for the Gas-Phase Oxidation of Methanol

**Fundamentals of Interfacial Phenomena III**
***Hilton San Francisco, Union Square 13***
• Effect of Photoisomer Composition in a Photoresponsive Surfactant System
• Fundamental Study of Adsorption Behavior of Ethoxylated Nonionic Surfactants from Organic Solvents on Various Surfaces
• Interfacial Rheology and Structure of Straight-Chain and Branched Fatty Alcohol Mixtures
• Monte Carlo Simulation of Lennard-Jones Surfactant Adsorption at the Liquid/Vapor Interface: the Effect of Tail Attractions, Temperature, Added Hydrophiles, and Surfactant Configuration
• Visualization of Cooperativity in the Building of Mixed Self-Assembled Monolayers
• Ionization, Molecular Recognition, and Wetting Phenomena on Self-Assembled Interfaces Formed from Chiral and Achiral Macrocylic Compounds
• Characteristics of Progeny Droplets Produced by Charge Instability Induced Breakups of Droplets

**Gene Therapy and Delivery (II)**
***Hilton San Francisco, Continental 8***
• Immunization Via Skin Using Vaccine-Coated Microneedles
• Construction of Hybrid Viral/Synthetic Gene Delivery Nanovectors
• Using RNA Interference to Probe Mechanism: DNase II Is Not Rate Limiting in Non-Viral Gene Transfer to Endothelium
• EGF Ligands Decrease Retroviral Gene Transfer through Protein Kinase C-Delta
• Expression-Targeted Gene Therapy for the Treatment of Transitional Cell Carcinoma
• Analysis of Retroviral Decay: Protein and RNA Stability
• Engineering Outer Membrane Vesicles for Gene Delivery

**In Silico Systems Biology I**
***Hilton San Francisco, Continental 3***
• In Silico Design of Synthetic Tetracycline-Inducible Regulatory Gene Networks
• Cellular Biosynthesis Responds to Changing Nutrient Environments: Predicting *in Vivo* Behavior from *in Vitro* Models
• Design and Mathematical Modeling of a Quorum Sensing Based Synthetic Ecosystem with Applications to Competitive Mixed Cultures
• Theoretical Considerations and Computational Analysis of Polyketide Biosynthesis Pathways
• Identification of a Mechanistic Model of Calcium Crosstalk and Caspase Activation in Mammalian Apoptosis
• Clinical Mutations in the Epidermal Growth Factor Receptor and Relevance to Oncogenic Transformations: from Molecular to Systems Level Modeling
• Sensitivity Analysis of Mammalian Circadian Clocks

**In Silico Systems Biology III**
***Hilton San Francisco, Imperial B***
• Modeling the ErbB Signaling Network in MCF-7 Breast Cancer Cells and Analysis of Ligand-Dependent Responses
• Simulation of Non-Specific Protein-Mrna Interactions in the Eif4f Translation Initiation Factor Complex
• A General Model for Ultrasensitivity Arising from Single Protein Multisite Modifications
• Spatial Organization of EGF Receptors and Its

Implications for Signaling
• How T Cells Hunt for Antigen in Lymphoid Tissue
• From Ligand Binding to Transcription Activation: *in silico* Simulation of Tumor Necrosis Factor-Induced Nuclear Factor Kappa B Activation Using Ibrena Software Package
• Antigen Quality Regulates Signaling and Degradation in the Immunological Synapse

### Inorganic Membranes for Gas and Vapor Separation
***Hilton San Francisco, Yosemite C***
• Permeation and Separation Characteristics of Silicalite Membranes on Zirconia Intermediate Layer by Template-Free Secondary Growth Method
• Mass Transport through Zeolite Membranes: Investigating Framework Polarity
• Small Pore Zeolites as Materials for Gas Separation Membranes
• Surface Modification of Pd Membranes with Cu
• The Preparation and Characterization of Hydrotalcite Membranes

### Integrated Design and Operation for Sustainability
***Hilton San Francisco, Continental 6***
• A Chemical Process Design Framework Including Different Stages of Environmental, Health and Safety (EHS) Assessment
• Qsar Approach for Mixture Toxicity Prediction Using Independent Latent Descriptors and Fuzzy Membership Functions
• Analysis and Decision Making for Sustainable Development of the Surface Finishing Industry
• Risk-Based Design of Metal Degreasing Process and Operation Considering Local Chemical Risks and Environmental Impacts
• Combining Expert System with Process Simulation for Waste Minimization in Batch Plant Operation
• Integration of Process Design and Operation with Implementation of a Kilo-Plant
• The Development of Energy Sharing in Industrial Areas of Japan with Pinch Technology

### Invited: in Honor of Massimo Morbidelli, Wilhelm Award Recipient II
***Hilton San Francisco, Imperial A***
• Optimizing Control of Simulated Beds
• Modeling Sorption and Swelling Behavior in Non-Equilibrium Polymer Phases
• Discontinuous and Continuous Operating Modes in Preparative Chromatography
• Visualization and Degree of Reproducibility of the Onset of Viscous Fingering in Chromatographic Columns
• Continuous Chromatography for Protein Purification

### Microfluidics and Small-Scale Flows I
***Hilton San Francisco, Union Square 15 & 16***
• Electro-Osmosis at Liquid-Liquid Interfaces
• Particle Manipulation on a Chip Using Conventional and Traveling-Wave Dielectrophoresis
• Dynamic Assembly in Nanochannels Manipulated by Electrokinetics
• Surface-to-Surface Transfer Printing of Liquid Inks
• Deflection Stability of an Electrohydrodynamic Liquid Bridge
• Transport of Cells and Particles through Ridged Polymeric Microstructures: Continuous-Flow Electrodeless Dielectrophoresis at Low Applied Electric Fields
• Flow between a Cavity and a Flexible Wall: Lubrication Model and Finite-Element Calculations
• Design and Testing of a Microfluidic Four-Roll Mill Device
• Modeling PCR in Natural Convection Systems
• Taylor Dispersion in Pcr in a Microchannel

### Molecular Simulation of Adsorption II
***Hilton San Francisco, Sutter***
• Design of Organically Modified Silicas for Carbon Dioxide Adsorption
• Simulation of Adsorption in a Modified Zeolite Y Used for Separating Chiral Compounds
• Molecular Simulation of Liquid Phase Adsorption of Chain Molecules in Zeolites
• Selectivities for Binary Mixtures of Hydrogen/Methane and Hydrogen/Carbon Dioxide in Silicalite and ETS-10 by Grand Canonical Monte Carlo Techniques
• Determining Contact Angles from Molecular Simulation
• A Molecular Dynamics Investigation of the Relative Stability of Alkaline Earth Metal-Chloride Complexes in Aqueous Solutions and on Gibbsite Surfaces
• Molecular Simulation of Water Adsorption in Silicalite: Effect of Silanol Groups and Different Cations

### Multiscale Modeling and Characterization of Polymers
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Semi-Grand Canonical Monte Carlo (SGMC) Simulations to Interpret Non-Equilibrium Polymer Melt Experiments
• Monte Carlo Simulations of the Interlamellar Region in Semi-Crystalline Isotactic Polypropylene
• Entanglements and Underlying Topology in Polymer Melts : from Atomistic Models to Entanglement Networks
• Spinodal Decomposition of Rodlike Liquid Crystals
• Molecular Modeling of Entanglements in Macromolecules by Using a Coarse-Grained Slip-Link Model
• Movement Selection for Modeling Biopolymers in a 3-D Lattice
• Diffusion in Polystyrene: a Multi-Scale Approach

### Nano-Scale Modeling of Interfacial Systems
***Hilton San Francisco, Continental 1***
• Brownian Dynamics Simulations of Polyelectrolyte Adsorption Onto Charged Patterned Surfaces
• Microscopic Properties of the Electric Double Layer at Metal Oxide Surfaces and the Effect of Hydrogen Bonding
• A Molecular Dynamics Study of Superspreading
• Quantitative Measurements of Colloid-Surface Interactions from Microscopic Imaging and Inverse Density Functional Theory
• Molecular Modeling of Transport across Surfactant Covered Oil Water Interface: Effects of Solute and Surfactant Properties on Transport Mechanisms
• Molecular Approach for the Design of Hydrofluoroalkane-Philes for Pressurized Metered-Dose Inhaler Formulations
• Monte Carlo Simulation of Chemical Reaction Equilibria at Modified Vapor-Liquid Interfaces

### National Science Foundation Workshop II
***Hilton San Francisco, Plaza A***
• Introduction - Workshop 2
• Overview of Chemical, Biochemical, Environmental, & Transport Division
• Catalysis and Chemical Processes
• Interfacial, Transport, and Separation Processes
• Fluids, Hydraulics, and Multiphase Systems
• Question & Answer Session II
• Thermal Systems (Thermal Processing & Combustion)
• Biochemical and Biomedical Engineering Programs
• Environmental Engineering and Technology
• Energy and Sustainability Activities
• Question & Answer Session and Panel Discussion

### Novel Adsorbent Materials and Structures II
***Hilton San Francisco, Powell***
• Molecular Modeling of the Adsorption of Small Molecules in Metal-Organic Frameworks
• The Interaction of Water with Metal Organic Framework-5 Simulated by Molecular Dynamics Using a New Non-Bonded Forcefield
• Mercury Adsorption on Activated Carbon
• Adsorption Equilibrium and Kinetics of Nitroaromatic Dye Removal: Comparing Vegetation-Polymer Beads and Activated Carbon
• Microfibrous Supported Catalysts/Sorbents: Novel Heterogeneous Contacting Systems with Enhanced Reaction Rates
• Carbon Replica from Silica Template Using Grand Canonical Monte Carlo Simulations
• Design of a Dual Purpose Air Filter for Semiconductor Clean Rooms

### Novel Computational and Experimental Methods in Multiphase Mixing
***Hilton San Francisco, Union Square 23***
• Correlation Equation of Particle Collision Frequency with Impeller in a Stirred Tank
• Computation of Interfacial Area Concentration Distribution in Bubble Columns
• Computational Flow Modeling of Multiphase Flow in Microfluidic Devices and Capillaries
• Simulating Fluid-Structure Interaction for Mixing Device Design
• Using a Macroscopic Particle Model for Dilute Solid Suspensions
• A New Methodology to Measure the Solids Dispersion in High Pressure Slurry Bubble Column Reactor

### Paradigms in Systems Biology (Invited)
***Hilton San Francisco, Grand Ballroom A***
• A Synthetic Approach to Systems Biology
• Mother Nature as Both Doctor and Patient

### Particle Technology Forum Award Lectures
***Hilton San Francisco, Continental 2***
• Particle Technology Forum Award Lecture

### Polymer Processing and Rheology III
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Using Computational Fluid Dynamics to Study Effects of Fiber on the Air Flow from an Annular Melt Blowing Die
• In-Mold Coating for Thermoplastic Substrates: Flow Modeling and Rheology
• Modeling of Morphological Development in Polyimide Microspheres Obtained from Powdered Precursors
• Aspects of Foam Injection Molding a Thermoplastic Polyolefin with Chemical Blowing Agents
• Understanding Polymer Nanofiber Electrospinning: Kinematic Measurements and Dimensional Analysis
• Melt Electrospinning of Polycaprolactone
• Polypropylene Film Casting

### Polymer Thin Films and Interfaces III
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Investigation of Block Copolymer Behavior on Patterned
• Symmetry Breaking in Block Copolymer Thin Films
• Self Assembly of Rod-Coil Block Copolymers and Homopolymers
• Self-Assembly of Double-Gyroid Phase Block Copolymer/Silica Thin Films
• Selectively Probing the Glass Transition Temperature in Block Copolymer Films
• Self-Assembly of Thin Polymer Film Via Electrohydrodynamic Instabilities
• Effects of Flow and Interfacial Block Copolymer on Polymer-Polymer Adhesion

### Poster Session: Advances in Environmental Technology
***Hilton San Francisco, Grand Ballroom B***
• Probabilistic Risk and Reliability Analysis of Oil and Gas Exploration and Production in Sensitive Ecosystems
• Design Considerations on an Annular Plasma Reactor for $NO_x$ Mitigation
• Studying Water Quality by Corrosion & Scaling

Index with Changing the Method of Microorganisms Control in Cooling Towers
• Effect of Btex and Ethanol on Biodegradation of MTBE
• Carbon and Ceria Supported Transition Metals for Low Temperature Carbon Monoxide Oxidation
• Experimental Study of Supercritical Water Gasification Using Fine Carbon Suspended Glucose Solution
• Initial Adhesion of Methanosarcina Barkeri to Support Materials
• The Toxicological Impacts of Selected Ionic Liquids on Industrial Wastewater Treatment Bacteria
• Utilization of Computational Fluid Dynamics and Aqueous Organic Oxidation Experiments to Aid the Development of a Tubular High-Density Plasma Reactor
• Parametric Study of Light Intensity on the Growth of Chroogloeocystis Siderophila in a Photo-Bioreactor
• Effect of Surface Characteristics of Microorganisms in Anaerobic Sludge on Immobilization to Support Materials
• Investigation of Rapid ZnO Dissociation in an Aerosol Flow Reactor
• Chlorine Atom Concentration Determination Via Gas Phase Titration with Butane
• Selective Recovery of Tantalum from Refractory Metal Scrap by Chlorination
• Energy and Transformity Matrix Analysis for Correlating Environmental Pollution with Birth Defects
• Coupled Chemical-Transport Modeling for Material Leaching Behavior Assessment in Environmental Conditions
• Methodology for Zinc Fate Assessment in Saturated Soil Material: Comparison between Batch and Continuous Laboratory Experiments
• Development of Gis-Based Toxic Pollutants Concentration Prediction System in Various Environmental Media
• Microbial Dynamics and Bioreactor Stability in an Oil-Absorber-Bioscrubber System Exposed to an Alternating Sequence of 1,2-Dichloroethane and Fluorobenzene
• Analysis and Integration of Drain Systems and Watersheds with Phosphorus and Nitrogen Compounds
• An Integrated Bioreactor – Activated Carbon Adsorption and Polysulfone Hollow Fiber Membrane Cell Immobilization – for Co-metabolic Transformation of 4-Chlorophenol
• Selection, Preparation, and Performance of High Temperature Novel $CO_2$ Sorbents
• A Sequencing Batch Reactor Achieving Enhanced Nitrogen Removal from Municipal Wastewater through Bypassing Nitrite Oxidation - a Pilot Scale Study
• Corrosion Phenomena of Alloys by Supercritical Water Oxidation of Halogenated Hydrocarbon in Batch Reactor and Anti-Corrosive Continuous Reactor
• Mercury Emission Analysis of 1600-MW Coal-Fired Power Plant by Ontario Hydro Method and on-Line Continuous Emission Monitoring
• Synthesis and Characterization of Photocatalytic Fibers by the Controlled Growth of Column-Shaped Nanotitanosilicate
• Analysis and Retrofit Design of Wastewater Treatment Facilities Using Process Simulation Tools
• Hydrogen Production from Natural Gas Reforming in Gliding Arc Discharge
• Selection of Optimal Biorefinery Products and Production Pathways
• Reactivity of Catalyst-Suspended Slurry in Supercritical Water
• Investigation of Ecological Services Impacts from Biofuel Production
• Decomposition of Fructose in Presence of Hydrochloric Acid in Continuous Subcritical Water System: Formation of 5-Hydroxymethylfurfural, Levulinic, and Formic Acids
• Production of Amino and Organic Acids from Scallop Wastes Using a Continuous Type, Small Scale Apparatus Sub-Critical Water Extraction and Hydrolysis
• High Speed Chitin Producing on from Crab Shell Using Sub-Critical Aqueous Acetic Acid Solution
• Reactions of α-Olefins Added during the Fischer-Tropsch Synthesis over Cobalt Catalyst for Selective Synthesis of Diesel Range
• Mechanical Characteristics of the Catalyst-Suspended Chicken Manure
• High Speed and Efficient Methane Fermentation Process for Sewage-Sludge Pretreated Using Sub-Critical Water Technology
• Improvement of Methane Fermentation Process Using Immobilized Methanogens on Bamboo Charcoal
• Analysis of Suspended and Biofilm Atrazine Degrading Cells
• Biotreatment of Trace Levels of Pentachlorophenol in Aqueous Media with Trametes Versicolor
• Design of Life Support Technologies for Microgravity Performance
• Direct Pretreatment of Urine by Activated Carbon for Highly Compact Space Life Support System Water Recycling
• New DOC – an Integrated Membrane Process for Wastewater Reclamation in Advanced Life Support Systems
• Steam Gasification of Waste Sawdust for Production of Synthesis Gas
• [CL] Determination Via Gas Phase Titration with Butane

### Poster Session: Applied Mathematics and Numerical Analysis

***Hilton San Francisco, Grand Ballroom B***

• A Novel Method of Grid Generation for Finite Elements
• Predicting Reboiler Operations Using Fluid Dynamic Modeling
• Applications of Conformal and Number Theory to Problems in Percolation Crossing Probabilities
• Validation of a Multiple Input, Multiple Output Model of the Human Thermoregulatory System
• A Tri-Frame Code Controls Entropy and Expression Levels of Proteins
• Computer Applications in Mineral Process Engineering - a Case Study in Mechanical Operations
• The Functionalities of Fast-Chrom/Smb (Fast and Accurate Simulation Tools for Chromatography and Smb)
• Joule Heating Effect on the Hydrodynamic Behavior of Eyring Fluids and on the Relative Importance of the Driving Forces

### Poster Session: Computers in Operations and Information Processing

***Hilton San Francisco, Grand Ballroom B***

• Identification of Supply Chain Relationships and Their Multi-Level Programming-Based Modeling
• Application of Tabu Search to Metabolic Flux Analysis Based on Labeling Balances
• Automatic Synthesis of Fuzzy Diagnosis Rules for Identifying Multiple Faults in Chemical Processes
• Production Planning and Scheduling Practices in the Pharmaceutical and Specialty Chemical Industries
• Superstructure-Based MINLP Formulation for Synthesis of Semi-Continuous Mass Exchanger Networks
• Flexible Inventory Management for Crude Oil Scheduling Problem
• Modeling of Purchase and Sales Contracts in Supply Chain Optimization
• Steel Scrap Purchasing Optimization and Supply Management
• Ontology Design and Its Application in the Gasification Domain
• Global Optimization of Multiphase Flow Networks in Oil and/or Gas Production Systems
• Data-Driven Soft Sensor Design with Multiple-Rate Sampled Data: a Comparative Study
• Assessment of Traditional Key Performance Indicators for Supply Chain Management in the Batch Chemical Industry
• A Computer Aided Approach to HAZOP Based on Functional Models
• Fiber-Optical Mid-Ir Spectroscopy for Chemical Processes
• Evaluation of the Pure Component Parameterization Methodology on Mixture Property Predictions for Thermodynamic Equations of State Using Terrain Methodology
• Comparative Assessment of Clustering Techniques for the Analysis of Temporal Gene Expression Data
• Large-Scale Multi-Vehicle Dispatching Problem for Chemical Products
• Automating the Analysis of Preprocessing Techniques for Chemometrics
• An Effective Transformation for Enhancing Stochastic Global Optimizations
• Scheduling of Parallel Furnaces Shutdown under Uncertainty
• Optimization of an Ideal Reactive Distillation Column Using Hybrid Integer Particle Swarm Optimization Algorithm
• Process Chemometrics at the Dow Chemical Company
• A Hybrid Tabu-Branch&Bound Approach for the Solution of Large-Scale Supply Chain Management Models
• A Population-Based Probability Distribution Estimation Method for Dynamic Optimization
• State Estimation in Constrained Nonlinear Systems - the Constrained Extended Kalman Filter
• Dynamic Data Reconciliation Using Process Simulator and Wavelet Denoising
• Integrating Multi-Variate Image Analysis and Artificial Intelligence Techniques with PVM for Inline Crystal Size and Shape Measurements
• Latent Variable Methods for Process Design: Dealing with Specification and Operational Constraints
• Implementation of an Experimental Platform for Chemical Process Integrated Operations
• Troubleshooting Supply Chain Systems with Procurement Rule Fortification/Restructuring
• Optimal Discharge Profile for Effective Utilization of Electrochemical Power Sources
• Development of Systematic Tuning Procedures for Extended Kalman Filtering

### Poster Session: Recent Developments in Systems and Process Control

***Hilton San Francisco, Grand Ballroom B***

• Control System Design for External Insulin Injection: a BMI Optimization Approach
• Optimal Identification in Systems Biology. Applications in Cell Signaling
• Optimizing DNA Plasmid Productivity from E. Coli Fermentation
• Dynamic Modeling and Analysis of Oxygen Enriched Coal Fired Boilers
• A Novel Method of Modeling Simple Thermodynamic System: a Case Study of a Tank Model
• Modeling of a Three-Phase Industrial Batch Reactor Using a Hybrid First-Principles Neural-Network Model
• Enhancing Fault Diagnosis by Incorporation of Intelligent Filtering Knowledge
• Integration of Data Rectification and Incipient Process Fault Diagnosis
• Design and Control of Isopropyl Alcohol Dehydration Via Homogeneous Azeotropic Distillation Using Dimethyl Sulfoxide as Extractive Agent
• Automatic Verification of Control Logics in Safety Instrumented System for Chemical Industrial Processes
• Multidimensional Modeling of Reactive Drying of Polymeric Films: an Integrated Process and Product Approach
• Disturbance Modeling Via Hidden Markov Techniques - an Extension
• A Novel Internal Cascade Structure for Control of Non-Self Regulating (Integrating) Processes
• Diagnosing Process Events Using Pattern Based Analysis of Control Data Metrics
• Continuous-Time Prediction-Error Identification for Mpc
• MPCA for Monitoring Emulsion Polymerization Process: Alternative Strategies for Decomposing

Three-Way Data Matrices
• Independent Component Analysis for on-Line Monitoring of an Emulsion Polymerization Reactor
• Interpolated Controller of a Fixed-Bed Reactor with Cold-Shot Cooling
• Verification of Fault Trees for Safety Integrity Level Evaluation in Hydrogen Processes
• Integrals of Relay Feedback Responses for Extracting Process Information
• Plant-Wide Control of HDA Process for Improved Profitability
• Fuzzy Steady State Decomposition Based Multi Model Control of Nonlinear Processes Applied to pH Control
• Optimal Experiment Design in Systems Biology
• Stochastic Modeling of Genetic Toggle Switch and Noise-Induced Transitions
• Modeling Crystal Size Distributions in Simulink

### Poster Session: Recent Developments in Systems and Process Design
***Hilton San Francisco, Grand Ballroom B***
• Conceptual Design and Simulation of a New Operation Mode for Reactive Batch Distillation Columns
• A Systematic Approach to Synthesize Optimal Operating Procedures for Transferring Materials in Batch Plants
• Development of a Mathematical Programming Model for Integrated Water Network Design in Batch Processes
• Analytical Flash Derivatives and Its Applications
• PLS Based Iterative Learning Control Scheme for Batch Systems
• Feasibility Measure Studies on Chromatographic Purification of Antibody Fragment from Clarified Lysate
• A Methodology Supporting the Design of 4-Section and 5-Section Jo Systems in Multicomponent Separation. I-Case of Linear Adsorption
• A New Algorithm for Bioprocess Feasibility Index under Uncertainty
• Increasing the Efficiency of Mass and Heat Exchange Networks
• Investigating the Need of a Pre-Concentrator Column for the Isopropyl Alcohol Dehydration Process
• Process Alternative for Methyl Acetate Conversion Using Reactive Distillation: Transesterification Versus Hydrolysis
• Process Integration Strategies for Optimization of Biocide Usage and Discharge for Seawater Cooling
• Equivalent System Mass Analysis and Integration of Food Production for Planetary Habitation
• Property Based Experimental Design
• Property Clusters and Group Contribution for Simultaneous Process and Molecular Design
• Multi-Objective Optimization under Uncertainty for the Sustainability Enhancement of Chemical Process
• Source Scale-up for Physical Vapor Deposition of Cu(InGa)Se2 on Flexible Substrates
• Development of a Design Algorithm for Petyluk Columns Using a Process Simulator
• Water Minimization in a Mixed Batch and Continuous Process Using Pinch Analysis Techniques
• Selecting Third-Party Logistics Contracts for Chemical Companies
• The Isothermal Reactive Flash Problem
• CFD Model for Performance Analysis of Nonwovens Absorbent Media
• Efficient Procedures for Nonlinear Sensor Network Design and Upgrade

### Property Estimation and Modeling for Product Design
***Hilton San Francisco, California Room***
• Dimensionality Reduction of Molecular Descriptor Matrices
• Liquid Densities of Petroleum Fractions: Revisiting the Peneloux Shift for Cubic Equations of State
• Rigorous and Exact: the "What Not to Teach" of Product Design
• The Range of Product Properties Predictable with Cosmotherm
• Rigorous and Exact: the "What Not to Teach" of Property Estimation
• Unified Physical Property Estimation Relationships-Upper
• Prediction of Glass Transition Temperature Using Hybrid Neural Networks
• Speadmd Correlation and Prediction of Transport Properties to Facilitate Chemical Process and Product Design
• Multiscale Property Modeling for Design of Polymer Based Products
• A System for Thermophysical Data Analysis and Optimization

### Reaction Path Analysis II
***Hilton San Francisco, Franciscan A***
• Isotopic Experimental and Modeling Study of Acetylene Formation in an a.C Plasma Reactor Using a Corona Discharge
• Kinetics of Selective Co Oxidation in Hydrogen-Rich Streams over Pt-Co-Ce/$Al_2O_3$ Catalyst
• Microkinetic Model for the Water Gas Shift Reaction on Supported Copper Catalyst
• Kinetic Modeling of the Isomerization and Alkylation Reaction Paths Involved in the Synthesis of Linear Alkylbenzenes over Y Zeolites
• Single-Event Microkinetics of Aromatics Hydrogenation on a Pt Catalyst
• Two Rate Determining Step Mechanistic Kinetic Model for Hydroisomerization and Hydrocracking of Long Chain Paraffins
• A Graph Theoretic Approach to Methanol Decomposition Reaction Mechanism and Kinetics
• Severe Pyrolyses of C6 to C12 Monocycloalkanes

### Reactions in near Critical and Supercritical Fluids II
***Hilton San Francisco, Union Square 5 & 6***
• Catalytic and Homogeneous Gasification of Biomass Model Compounds in Supercritical Water
• Kinetic Modeling and Mass Transfer Effects in Homogeneous Catalytic Hydroformylation of 1-Octene in $CO_2$ – Expanded Solvent
• Hydrolysis Kinetics for 2,3-Dichloropyridine in Supercritical Water
• Catalysis, Phase Equilibria and Mass Transport for Hydrogenation and Hydroformylation in Biphasic Ionic Liquid-Compressed $CO_2$ Systems
• Melt Glycolysis of Poly(Ethylene Terephthalate) Using $CO_2$-Assisted Extrusion
• Highly Active and Recyclable Hydroformylation Catalysis Using Phase Controlled Polymer Supports in $CO_2$-Expanded Liquids (Cxls)

### Sensing Applications of Nanocomposites
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Effect of Foaming on Fiber Orientation and Electrical Conductivity of Polymer Carbon Fiber Composites in Injection Molding
• Negative Normal Stresses in Polymer Nanocomposites
• HDPE/$Al_2O_3$ Nanocomposites Prepared by Extruding $Al_2O_3$ Coated HDPE Particles
• Large-Scale Production of Carbon-Coated Copper Nanoparticles for Sensor Applications
• Film Characteristics of Magnetic Nanoparticles Incorporated into Tethered Thermoresponsive *n*-Isopropylacrylamide Copolymer Hydrogels
• Responsive Polydiacetylene/Silica Nanocomposite Films with Tunable Mesostructure and Thermochromatism
• Uv-VIS Properties of ZnO / Low Density Polyethylene Nanocomposites
• Responsive Nanocomposites Though Hierarchical Assembly

### Size Effects in Catalysts at the Nanoscale
***Hilton San Francisco, Franciscan C***
• Nano-Scale Effects in the Oxidation and the Reactivity of Platinum Clusters
• Effect of Pt Cluster Size on the Reaction of No and $O_2$ to $NO_2$ on Supported and Model Catalysts
• Stabilization of Platinum Nanoparticles by Substitutional Boron Dopants in Carbon Supports
• On the Activity of Cationic Au Species during the Preferential Co Oxidation on Low Content Au/$CeO_2$Catalysts
• Synthesis and Characterization of Dendrimer-Derived Ir/-$Al_2O_3$ Catalysts
• Performance Testing and Structural Characterization of Gamma-$Al_2O_3$-Supported Rhenium Clusters and Particles for Methylcyclohexane Conversion
• Sol-Gel Synthesis of Vanadium Phosphorus Oxides as Catalyst for the Partial Oxidation of Butane to Maleic Anhydride

### Thermodynamic Properties and Phase Behavior V
***Hilton San Francisco, Union Square 19 & 20***
• Salt-D: a New Equation of State for Polymeric Fluids
• Thermodynamically Constrained Inverse Monte Carlo: Potentials Optimized to Reproduce Structure and Thermodynamics
• A New Approach for Calculation of Minimum Miscibility Pressure Based on a Multiple-Mixing-Cell Model
• High Accuracy Density Measurements at Pressures up to 200 Mpa for Light Synthetic Natural Gas-like Mixtures
• Perturbation Thermodynamic Theory for Polar Fluids: Pure Components and Mixtures
• The Nature of Asymmetry in Fluid Criticality
• Gas and Volatile Organic Compound Partitioning in Aqueous Environments
• Thermodynamic Properties of Humid Gases from First Principles

### Thermodynamics under High Pressure
***Hilton San Francisco, Union Square 14***
• High Pressure Phase Behavior of Binary Systems of Refrigerants and *n*-Alkylbenzenes
• Vapor-Liquid-Liquid Equilibria of Ternary Fluorous, Organic, and Carbon Dioxide Systems
• The Use of Tetrahydrofuran to Stabilize the Clathrate Hydrates of Helium, Neon and Hydrogen at Low-Pressure
• Formation of Mixed Gas Hydrates: a Thermodynamic Study
• Thermodynamic Modeling of High Pressure Gas Storage System
• Thermophysical Property Predictions of the Opls-Aa, Trappe-Ua and Borodin Force Fields for Perfluoroalkanes
• The Isothermal Compressibility Peaks in Hydrogen Fluoride in the Super Critical and Super Heated Vapor Region

### Thermophysical Properties of Biological Systems III
***Hilton San Francisco, Union Square 1 & 2***
• How Attractions Affect the Collapse of a Hydrophobic Polymer in Water
• Computing Free Energies of Bound Water in Confined Environments and at Interfaces
• Solvation Free Energy of Amino Acids and Side-Chain Analogs
• Thermodynamic Analysis of Interacting Nucleic Acids with Application to Biosensing Devices
• Simulation of pH-Dependent Edge Strand Rearrangement in Human B-2 Microglobulin
• Computational Predictions of Protein-Protein Structures and Interfaces within a Messenger RNA Degradation Machine
• Evaluating Free Energy Changes during Protein Adsorption Processes
• A Comparative Thermodynamic Study of the Interactions of Human Stratum Corneum and Its Components with Water

### Turbulent Flows
***Hilton San Francisco, Union Square 17 & 18***
• Scalar Transport in Turbulent Flows over Com-

plex Surfaces
• Temperature and Number Density Measurements Using Raman Spectroscopy in Supersonic, Turbulent, Combusting Flows
• A RANS Model for Turbulent Drag Reduction by Polymer Injection
• Mechanisms of Particle Dispersion and Concentration in Unsteady Virtual Impaction Jets
• Validation of LES Simulation of a Large Helium Plume
• A Novel Two-Phase Filtered Density Function Approach for Turbulent Spray Combustion
• Experimental Study of Turbulent Reactive Mixing in a Confined Rectangular Jet Reactor
• Realizable Algebraic Reynolds Stress Model for Single Phase and Multiphase Turbulent Flows
• Multi-Environment Conditional Pdf Model Validation Study Using Reacting Flow Dns
• Spectral Mixing Model for the Composition Pdf of Inhomogeneous Scalar Fields in Isotropic Turbulence

**TUESDAY, 14 NOVEMBER 2006**
***6:00 PM - 7:00 PM***
**Professional Progress Award Lecture**
***Hilton San Francisco, Grand Ballroom A***

**TUESDAY, 14 NOVEMBER 2006**
***6:30 PM - 9:00 PM***
**AES Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Blood Typing in a Dielectrophoretic Microdevice
• Lab-on-a-Chip Sample Preparation for Subcellular Analysis: a Technique to Rapidly Rupture Erythrocytes in a Dielectrophoretic Microdevice
• Lessons Learned from "Not Entirely Successful" Attempts to Use Room Temperature Ionic Liquids (RTILs) for Electrochemical Separations

**General Poster Session on Separations**
***Hilton San Francisco, Grand Ballroom B***
• Hydrodynamic Instabilities in Cyclone Separators of Small Scale
• Mixed Matrix Membranes for Gas Separation
• Carboxylic Acid Effects on Ethanol Recovery from Aqueous Mixtures Using Pervaporation through MFI Zeolite-Filled Polydimethylsiloxane Membranes
• Modeling and Simulation of Oil-Water Separation Using Subsea Equipment
• Olefin/Paraffin Separation Using a Mesoporous Material
• A General Strategy for Adhesion Enhancement in Mixed Matrix Membranes by Formation of Nano-Structured Particle Surfaces
• Singularities in Modeling Reactive Flash Systems
• Colloidal Templating with Surface-Anisotropic Particles
• High Temperature Carbon Dioxide Capture and Hydrogen Production Using Engineered Eggshells
• Modeling Swirl Flow at Different Viscosities
• Ion Exchange Adsorption Process for *in Situ* Removal of the Unstable ß-Lactamase Inhibitor Clavulanic Acid from *S. Clavuligerus* Fermentation Broth
• Reverse Micelle Extraction of EGFP

**Poster Session in Fluid Mechanics**
***Hilton San Francisco, Grand Ballroom B***
• The Economical Fabrication of Surface-Directed Microfluidic Platforms and the Characterization of Capillary Dynamics
• Transport Properties of Electrospun Nanowebs
• Geometrical Effects on Helical Flow in Grooved Microchannels
• Computation Fluid-Dynamics Modeling of a Microfluidic Cell Separation Device for Cardiac Tissue Engineering
• Computational Particle Fluid Dynamics Simulations and Validation for Cyclones: High and Low Loadings
• Large Particle Detachment in a Microchannel
• Two-Phase Flows in Microfluidic Devices
• Surface-Mediated Drop Motion in a Bifurcating Microchannel with Different Wettabilities
• Dimensional Analysis of Steady and Unsteady State Permeation Flux for Microfiltration of Oil/Water Emulsion by a Ceramic Membrane
• Microstructure & Rheology of Thixotropic, Shear Thickening Dispersions
• Thermocapillary Induced Motion of a Drop with Simultaneous Effect of Surface Viscosity
• Passive Single Droplet Dispensing Using Capillary on EHD Method
• Open-Channel Capillary Flow in Minimal Support Structures
• Studies on Mass Transfer Using Co-Axial Orifice Turbulence Promoters
• Hydrodynamic Interactions of Spherical Particles between Two Planar Walls: Accelerated Stokesian-Dynamics Algorithm
• Numerical Simulation of the Confined Motion of Drops and Bubbles Using a Hybrid VOF/Level Set Method
• Creeping Motion of a Sphere in a Cylindrical Conduit
• Experimental and Theoretical Study of Suspensions of Magnetic Nanoparticles in an Annular Gap Subjected to a Rotating Magnetic Field
• Comparison of Experimental Results and Model Predictions for Complex Geometry Flows of a Concentrated Suspension
• Particle Migration in Stokes Flow of Suspensions past a Cylinder
• Flow of Suspension past a Cylinder at Low Reynolds Number
• Flows of Concentrated Suspensions in Symmetric and Asymmetric Bifurcations Measured by NMRI
• Nature of Hemodynamic Forces on Vascular Endothelial Cells, Leukocytes or Cancer Cells Adhering to the Surface of Blood Vessels
• Dynamics of DNA Tumbling in Shear and Rotational Flows
• Coating Flows on a Rotating Vertical Disc
• The Effect of Non-Newtonian Fluid and Flow Conditions on the Instability of an Annular Liquid Sheet
• Comparison of Numerical and Taylor-Based Solutions for Power-Law Model Fluids with Joule Heating in a Rectangular Capillary Cell
• Asymptotic Analysis of the Selective Dip-Coating of Power-Law Fluids Onto Chemically Micropatterned Surfaces
• Lateral Expansion of Thin Dough Sections under Sudden Pressure Release
• Rheological Behavior of HDPE-Wood Flour Composites Manufactured in Different Flow Field
• Experimental Study on Polymer Melt Flow in Water Assisted Injection Molding
• A Three-Dimensional Lattice Boltzmann Simulation of Non-Newtonian Fluid Undergoing Extremely High Shear Rate in the Confined Geometry
• Blood Flow Patterns in the Carotid Artery and the Risk of Atherosclerotic Diseases
• Using Rheological Properties of Body Fluids as Physiological Indicators
• An Axisymmetric Single-Path Model for Reactive Gas Transport and Uptake in the Conducting Airways
• Controlling Wall Turbulence by Modifying the Channel Wall
• Blood Flow Analysis in Micromed Debakey Pump by Computational Fluid Dynamics
• The Onset of Turbulence in Drag-Reducing Aggregated Polymer Solutions
• Computational Fluid Dynamic Simulation of a Multiphase Fluid in Vertical Flow at High Reynolds Number

**Poster Session on Membranes**
***Hilton San Francisco, Grand Ballroom B***
• Effect of External Recycle on Extraction in Rectangular Membrane Modules
• Stability Study of Hollow Fiber Membrane in Olefin/Paraffin Separation
• Synthesis of Fluorine-Containing Polyimides for Pervaporation Separation of Toluene/*n*-Heptane Mixtures
• Effect of Intercrystalline Pores in MFI Zeolite Membranes on Xylene Separation and Membrane Improvement by Online Coking
• Designing Adsorptive Membranes Using Confocal Microscopy
• Transient Permeation of Binary and Ternary Gas Mixtures on MTES Templating Silica/á-Alumina Composite Membrane
• Asymmetric Carbon Molecular Sieve Membranes Based on Poly(Phenylene Oxide) for Gas Separation
• New Approach to Improve Gas Permeability through Amorphous Glassy Polymer Membranes
• Enhancing Flux for Membrane Distillation
• Transport Properties of Proton Exchange Membranes: Effect of Supercritical Fluid Processing
• Mathematical Modeling for Transdermal Transport of Volatile Organic Liquids
• Selectivity of Affinity Membranes for Immunoglobulin Capture
• New Tubular, Composite Membranes for Air Removal from Aerospace Fluid Loop Coolant Systems
• Fabrication of Cylindrical Micro-Porous Membrane Via Utilization of Colloidal Templating
• Enhancement of Whey Protein Filtration Using Modified Polyethersulfone(PES) Membranes
• Ordered Mesoporous Silica Membranes: Preparation and Nanopermporometry Characterization
• Synthesis and Characterization of Silica Sodalite Membranes Obtained by *in-Situ* Crystallization and Secondary Growth Methods
• The Effect of Metal-Catalyzed Oxidation on Diffusion in Polybutadiene
• Performance of Homogeneous and Heterogeneous Ion-Exchange Membranes during Donnan Membrane Process Based Alum Recovery
• Transient Diffusion of Gases in Polymer Foams Having Non-Uniform Density
• Gas Diffusion in Polystyrene Film
• Thermodynamics and Dynamics of Water Vapor Sorption in Thin Polymer Films
• Characterization of Phosphoric-Acid-Doped Polybenzimidazole/Cesium Hydrogen Sulfate Composite Polymer Electrolyte Membranes for Fuel Cells

**Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange**
***Hilton San Francisco, Grand Ballroom B***
• On-Line Monitoring of Enantiomer Concentration by High-Speed HPLC in Multicolumn Continuous Chiral Chromatography
• *In-Situ* Probing of Insulin Aggregation in Chromatography Effluents with Spectroturbidimetry
• Characterization of Porous Sorbents by Simultaneous Measurement of Adsorption Isotherms and Enthalpies Using a Sensor Gas Calorimeter (SGC)
• Computational Fluid Dynamics Simulations of Adsorption Columns Based on Computed Tomography Experiments
• Studies in Continuous Countercurrent Pressure-Difference-Driven Gas Adsorption Separations
• Adsorptive Separation of Platinum Group Metals in Fixed-Bed Columns Containing Amine-Immobilized Activated Carbons
• Process Innovation in the Sugar Industry: Chromatographic Sugar Separation Using Smb Technology
• Scaling and Sensitivity Analysis of Simulated Moving Bed Reactors
• Chitosan Selectivity to Remove Cadmium (II), Copper (II) and Lead (II) from Aqueous Phase: pH and Organic Matter Effects
• Acid Activated Bamboo-Type Carbon Nanotubes and Cup-Stacked-Type Carbon Nanostructures as Adsorbent Materials: Cadmium Removal from Water
• Experimental Validation of the Hybrid Membrane/PSA Principle for Gas Separation
• Multicomponent Adsorption in Porous Media
• Production of 2,6-Dimethylnaphthalene Using a Simultaneous Isomerization and Adsorption Based

Reactive Adsorption Technique
• Steam Regeneration of Activated Carbon and Day Zeolite Adsorbed by VOCs
• Optimized High-Throughput Asynchronous Smb Process with Modulated Eluent Flow Rate and Pulsed Production
• On-Line Monitoring of an Optimized Enantioseparation by High-Speed HPLC in Multicolumn Continuous Chromatography
• Divinylbenzenes and Methacrylates Copolymeric Adsorbents for the Denitrogenation of Straight Run Gas Oils
• Effect of Selectivity on Partial Feed Operation for Four-Zone Simulated Moving Bed Chromatography
• Chromatographic Study of Multicomponent Gas Adsorption on Msc5a
• Adsorption of Organics on Msc5a in Supercritical $CO_2$,Molecular Simulation
• Adsorption of Mixed Organic Solvent by Y Type Zeolite
• Measurement and Molecular Simulation on Adsorption Equilibrium and Adsorption Kinetics of the Chlorinated Hydrocarbons into High Silica Zeolite
• Separation of Ditetrahydrofurylpropane by Adsorption in Conventional Adsorbents
• Study on Removal of Harmful Substance in Incineration Bottom Ash of Municipal Waste by Wet Process
• Uptake Characteristics of Monovalent Metal Ion Species by Tannin-Gel
• Adsorption Equilibrium of Multi-Solute Aqueous Solutions Onto Activated Carbon
• Study on Zeta-Potential of Adsorbent in Aqueous Solution - Activated Carbon Adsorption System
• Removal of Alkali Metals from Organic Solvent Containing Coal Extract at Elevated Temperature and Pressure Using Inorganic Ion Exchangers
• Intracrystalline Diffusivities of Linear Paraffins in Zeolite Beta Using ZLC
• CO2 Adsorption Utilizing Porous Microfibrous Media Entrapped Liquid $K_2CO_3$ as an Apparent Solid
• Molecular Simulation of Poliaromatics Adsorption in Mesoporous Molecular Sieves
• A Novel and Simple Method for Finding the Heterogeneity of Adsorbent on the Basis of Adsorption Kinetic Data
• Development of Carbon Monoxide-Selective Adsorbents for Rapid-Cycle Pressure Swing Adsorption
• Characterization Method of Micro-Gel Particles within Synthetic Resin Adsorbent
• Adsorption and Desorption Characteristics of Some Chlorinated Herbicides Onto Activated Carbon
• Adsorption and Desorption Characteristics of Some Chlorinated Herbicides Onto Activated Carbon
• Sterilization of Pathogenic Bacteria Using Titanium Dioxide Photocatalyst
• Influence of Acetic Acid on the Photovoltaic Performance of Ru(II) Dye Sensitized Nanocrystalline $Tio_2$ Solar Cells
• An Algebraic Modeling of Dual Reflux PSA Process for High Enrichment and Recovery of Dilute Adsorbate
• Study of the Adsorption of Hydrocarbons Mixture on Disabled FCC Catalyzer
• Molecular Simulation of the Adsorption of MTBE in Silicalite, Mordenite, and Zeolite Beta
• Adsorption of Chromium(VI) from Water Solutions on Activated Carbon Fiber
• Study on Packing Structures in Liquid Chromatography (LC) Columns Based on X-Ray CT
• Development and Scale-up Studies of a Smb Process for the Production of Citric Acid
• Adsorption and Mass-Transfer Behaviors of Amino Acids in a Fixed Bed Packed with PVP Resin
• Pinched Wave Design of an Smb for the Separation of Glucose and Fructose
• A Single Five-Zone Smb System for Complete Separation of Three Amino Acids Mixture
• Removal of Zinc and Iron from Aqueous Solution by Ion Exchange with Na-Y Zeolite
• Iteration Function Method for Mixture Adsorption Calculations

**Poster Session: Fundamentals and Applications of Extraction**
***Hilton San Francisco, Grand Ballroom B***
• Solid Phase Extraction for Heavy Metals Prior to Atomic Absorption Spectroscopy
• Sfe Extraction of Squalene from Oil Residues
• The Effect of Microwaving and Ultrasonication on the Yield and Product Profile of Jerusalem Artichoke Extracts

**Poster Session: Recent Developments in Crystallization and Evaporation**
***Hilton San Francisco, Grand Ballroom B***
• Formation of Low Acidity ADNBF by Reactive Crystallization
• Formation and Characterization of II-VI Semiconductor Nanocrystals
• Crystallization of Low Solubility Calcium-Arsenate Compounds for Poly(Diallyldimethyl Ammonium Chloride) Recovery from Peuf Retentate Streams
• Prediction for Solvent Effect on Crystal Morphology of an Energetic Material by Molecular Modeling
• Distribution of Impurities in Protein Crystallization
• Evaporative Crystallization of Sodium Sulfate Dicarbonate
• Nucleation of Lysozyme Crystals on Modified Substrates
• Solvent Effect on Morphology of Crystals

**Thermodynamics and Transport Properties (Posters)**
***Hilton San Francisco, Grand Ballroom B***
• An Extended CEOS/ AE Zero-Pressure Mixing Rule and Its Application to Phase Equilibrium Calculation
• Chemical Force Microscopy and Ab Initio Calculations: a Molecular Approach for the Design of Surfactants for Pressurized Metered-Dose Inhalers
• Hydrogen Storage by Adsorption Onto Different Activated Carbons
• Phase Behavior of Ionic Fluids in Disordered Charged Media
• Describing the Global Thermodynamic Properties of Chain Fluids Using a Crossover Perturbed-Chain Statistical Associating Fluid Theory
• Using Voronoi Tessellations to Measure Coexisting Densities for Molecular Dynamics Simulations
• Computing Thermophysical Properties of Aromatic Compounds: Comparison of Theory and Experiment
• Gas Solubility, Diffusivity, and Surface Tensions in Phosphonium-, and Ammonium-Based Room Temperature Ionic Liquids
• Computer-Aid Simulation of Gas Solubility and Diffusivity in Room Temperature Ionic Liquids – Initial Progress Report for Computer Aided Design of RTIL-Based Separating Agents
• Developing a New Equation of State with Non-Quadratic Mixing Rules for Prediction of the Phase Equilibria of Polar and Associated Fluids
• Coarse-Graining and Soft Matter Systems: Bridging the Atomistic-Meso Scales
• Prediction of $N_2$ and $CO_2$ Gas Hydrate Equilibria
• A Novel Separation Process of Gas Mixtures by Using Tetrahydrofuran (THF) Clathrate Hydrate
• Basic Study of Hydrogen Storage in THF/$H_2$ Clathrate Hydrate
• Nanocomposite Materials for High Capacity Hydrogen Storage
• Generalization of a Viscosity Model for Liquid Mixtures Using an Artificial Neural Network
• Prediction of Global Warming Potentials through Computational Chemistry – Testing Robustness of Methodology through Experimental Comparisons
• Development of Atomistic Force Fields for Binary Mixture Vapor-Liquid Equilibria Calculations
• Effect of Torsional Potential on the Phase Behavior of Organic Compounds
• Chemicals Regulation and the Integration of Process Safety with Molecular Modeling
• On Solubility Extrema in Solid-Fluid Equilibrium and the Effect on Thermodynamic Modeling
• Triangular Well Equation of State for Fluid Mixtures
• Equilibrium Properties from the Crossover Triangular Well Equation of State
• Compressed Liquid Densities for Binary Mixtures of [Emim] Chloride + 1-Butanol from 313 to 363 K and Pressures up to 25 Mpa
• Liquid Densities of Hexane + Benzothiophene Mixtures from 313 to 363 K and up to 25 Mpa
• Simulation of the Frictional Response of Nanoconfined Films
• Estimating Molecular Mobility in Amorphous Organic Pharmaceutical Compounds
• Temperature and Pressure Effects on Structural Properties of Supercritical Water Molecules Confined in Carbon Nanotube—-a Molecular Dynamics Study
• The Use of Hard-Core Two-Yukawa Potential in IMAC for Prediction of Diffusion Coefficients
• Transformation of Amorphous Titania to Anatase: Kinetics and Dynamics
• Monte Carlo Simulation of Fluid Systems at Fixed Entropy
• Solubility of Methane in Binary Mixed Solvents (Ethanol+Hexane Andethanol+Cyclohexane) at High Pressures
• Liquid-Vapor Isotopic Fractionation Factors of Diatomic Fluids. Simulation, Modeling and Comparison with Experiment
• Recent Advances with the Cubic – Plus – Association Equation of State
• Multiplicity of Correlation Functions in Fluids
• Applications of the Simplified Perturbed-Chain Salt Equation of State
• Revisiting Scaled Particle Theory of the Binary Hard Sphere Fluid
• Phase Behavior of Ionic Fluids in Charged Disordered Media
• Vapor-Liquid-Liquid Equilibria and Lower Critical Solution Temperatures of Hydrofluorocarbons in Room-Temperature Ionic Liquids
• Modeling of Aqueous Amino Acid and Polypeptide Solutions with Pc-Salt
• Critical Point Calculation of Lennard Jones Pure Fluid and Binary Mixtures
• The Influence of Ion Polarizability on the Electric Double Layer
• Ab Initio Monte Carlo Simulations of Fluid Phase Equilibria at Extreme Conditions
• A Conformal Equation of State for Carbon Tetrafluoride and Neopentane from Molecular Simulation
• Measurement and Correlation of Partition Coefficients of Sulfur Compounds for Acetonitrile + *n*-Alkane Systems
• Understanding the Phase Behavior of Aqueous Hydrogen Fluoride Mixture by Incorporating Self and Cross Association Patterns
• Statistical Associating Fluid Theory Coupled with Restricted Primitive Model to Represent Brine/Seawater up to High Temperatures and Pressures
• Model for Solubility and Solid Phase Composition in High-Temperature $Na_2CO_3$-$Na_2SO_4$ Solutions
• Phase Equilibria for Bio-Derived Chemicals
• Equation of State Modeling of Polarizable Dipolar and Quadroupolar Mixtures
• Atomic-Scale Analysis of Silicon Hydride Dissociation on Surfaces of Plasma-Deposited Amorphous Silicon Thin Films
• Predicting the Lennard Jones Melting Point, Infinite Size and Full Potential
• Melting Transition in Repulsive Lennard Jones Crystals
• Equation of State for Lennard-Jones Fluid and Chains in the Npt Ensemble
• Volume-Explicit Equation of State for Square-Well Monomers and Chains
• Reliable Computation of Density Roots, Phase

Stability and Phase Equilibrium Using Salt Equation of State
• Estimation of Critical Points from the Virial Equation of State

**WEDNESDAY, 15 NOVEMBER 2006**
***8:30 AM - 11:00 AM***
**(22b) Nanoscale Science and Engineering in Biomolecular Catalysis I**
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Supramolecular Templating of Nanoporous Catalysts
• Hybrid Molecular Sieve Supported Biocatalysts
• Biomimetic Silica Encapsulation: an Efficient and Versatile Enzyme Immobilization Technique
• Preparation of Tuneable NPT Surfaces for Sensing and Biomedical Applications
• Unusual Interfacial Activation of Burkholderia Cepacia Lipase Immobilized in Nanopores of SBA-*15 Silica*
• Carbon Nanotubes Suspension for Biosensor Applications
• Dispersion of Polystyrene - Poly (Styrene-*Co*-Maleic Anhydride) Nanofibers in Aqueous Solutions for Biocatalytic Continuous Flow Reactors
• Proteins Assisted Dispersion of Carbon Nanotubes

**(22b) Nanotechnology for Biotechnology and Pharmaceuticals Industries**
***Hilton San Francisco, Sutter***
• *Ex-Vivo* Tissue Engineering in Inverted Colloidal Crystal Scaffolds with Nanostructured Surface Coating from Organic-Inorganic Composite
• Physicochemical Characteristics of Drug-Laden Nanofibers for Controlled Drug Delivery
• Synthesizing Core/Shell Nanoparticles for Magnetic Fluid Hyperthermia Cancer Treatment
• Towards the Large-Scale Chemical Self-Assembly Processing of Virus-like Particles
• Nanoparticle Delivery of Stabilized Angiogenic Growth Factors
• Conjugation of Fept Nanoparticles with Biological Entities
• The Design of Liposome-Based Anthrax Toxin Inhibitors

**(22b) Self-Assembled Biomaterials**
***Hilton San Francisco, Continental 8***
• Controlling Cell Interactions to Polyelectrolyte Multilayer Assemblies Based on Elastin-like Polymer Conjugates
• Room Temperature-Nanoparticle Synthesis Using Ring-Structured Peptide Assemblies as Templates
• Polymerization Control of Templated Recognitive Structures
• Investigating Antibody Access to Adsorbed Protein Nanocapsule Interiors Using the Quartz Crystal Microbalance and Surface Plasmon Resonance
• *Escherichia Coli*-Based Cell-Free Protein Synthesis of Virus-like Particles
• Self-Assembly and Nanoparticle Formation of a Novel Bioresorbable and Crosslinkable Terpolymer
• Thermally Reversible Heteroaggregation of Lipid Vesicles Using DNA as Biomolecular Combination Locks
• Vesosome – a Multicompartment Bilayer Structure Encapsulating Vesicles and Colloids
• Vesicles in Biopolymer Capsules: Hybrid Structures for Controlled Drug Delivery
• Engineering of Self-Assembled Phi29 Nanomotor for the Applications in Nanotechnology and Gene Therapy

**Advances in Adsorptive Bioseparations**
***Hilton San Francisco, Powell***
• Preparation of Ribonuclease A Surface-Imprinted Nanoparticles with Miniemulsion Polymerization for Protein Recognition in Aqueous Media
• Fundamental Studies on Dual Mode Biomolecular Separations in Ordered Mesoporous Materials
• Studies of Interactions of an Amylose-Based Sorbent with Various Solvents for Chiral Separation Applications
• Molecular Dynamics Modeling and Simulation of Chromatographic Bioseparation
• The Effect of Buffer Salt Species and Concentration on the Internal pH of a Strong Anion Exchange Resin
• Affinity Adsorption Chromatography Modulated by Polymer Permeation Control. an Strategy to Purify Peptides and Small Proteins
• Optimization of the Gradient Profiles for Multi-Component Separation in Reversed Phase Column

**Advances in Bioseparations**
***Hilton San Francisco, Yosemite B***
• Simple and Economical Purification of Recombinant Proteins by Self-Cleaving Aggregation Tags
• Molecularly Imprinted Polymeric Microparticles for Bio-Analytical Applications
• A Rational Method to Improve Bioseparation Via Proteomics
• A Proteomics Approach to Evaluate Expression Host and Downstream Recovery Compatibility: Analysis of Maize and Ion Exchange Chromatography
• Purification of Biomolecules by Multicolumn Countercurrent Solvent Gradient Chromatography (MCSGP)
• Purification of *E. Coli* Inner Membrane Vesicles by Biotin-Streptavidin Interaction
• Osmotic Second Virial Coefficient as a Useful Tool to Optimize Self Assembly of Virus-like Particles

**Advances in CE and Microdevice Technology for Genomic Analysis**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• How Is It Possible to Sequence 600 Bases of DNA in 6.5 Minutes? the Central Role of Carefully Engineered Polymer Networks and Coatings in Microchip Electrophoresis
• Nanostructural Characterization of Photopolymerized Polyacrylamide Gels for DNA Electrophoresis
• DNA Sequencing and Separation in Free Solution Using Engineered Drag-Tags
• Microchip-Based Electrophoretic Analysis of Low Abundant Unknown Mutations Using Site-Specific Nicking and Ligation Enzymes
• Sacrificial Layer Methods for Making High-Performance Capillary Electrophoresis Microchips
• Optimal Separation Times with an Orthogonal Electrical Field in a Cylindrical Capillary

**Advances in Energy R&D - Plant Operations Applications**
***Hilton San Francisco, California Room***
• The US Dept of Energy - Energy Efficiency & Renewable Energy's Industrial Technologies Program
• The U.S. EPA and DOE Energy Star Program
• Energy Regulatory and Funding Update
• Plant Energy Conservation Case Studies - Steam
• Plant Energy Conservation Case Studies - Process Heating
• Plant Energy Conservation Case Studies - Motors, Pumps and Fans
• Plant Energy Conservation Case Studies - Compressed Air

**Advances in Metabolic Engineering and Bioinformatics (I)**
***Hilton San Francisco, Continental 9***
• From Clustering Expression Data to Gene Network Reconstruction: Array Informatics Using Mathematical Programming
• Elementary Metabolite Units (Emu): a Novel Framework for Modeling Isotopic Tracer Distributions and Determining Metabolic Fluxes
• Strain Design by Reverse Engineering Enzyme Expression Levels from Metabolic Fluxes
• Reconstitute Biosynthesis of Tetracycline Intermediates
• Transcriptomic Studies of an Amorphadiene Producing *E. Coli* Strain in an *Acka/Pta/Poxb* Deletion Background
• Utilization of a Genetic Toggle in the Control of Poly(3-Hydroxybutyrate-CO-3-Hydroxyvalerate) Composition in Recombinant *Escherichia Coli*
• Metabolic Engineering of *E. Coli* for Alpha-Gal Epitope Synthesis
• Natural and Unnatural Flavonoid Biosynthesis and Their Insulinotropic Properties in Pancreatic Beta Cells

**Advances in Real-Time Optimization**
***Hilton San Francisco, Union Square 17 & 18***
• First-Order Robust Real-Time Optimization
• Coordinator Mpc for Maximization of Plant Throughput
• Mpec Formulations to Model Complementarities in RTO Problems
• Optimal Control of Partially Observable Markov Decision Processes

**Advances in the Pyroprocessing Based Fuel Cycle**
***Hilton San Francisco, Union Square 13***
• Study of Jet Splashing at Liquid/Gas Interface in an Oxide Reduction Electrochemical Cell
• Electrorefining of Reduced Spent Nuclear Oxide Fuel at Bench Scale
• Corrosion Study of an Oxide Dispersion Strengthened Nickel-Based Superalloy in a High Temperature $Li_2O$/LiCl Molten Salt under Oxidizing Conditions
• Effect of Salt and Zeolite Particle Size on Preparation of Salt-Loaded Zeolite in the Ceramic Waste Process
• Cesium and Strontium Separations for Pyroprocessing of Spent Oxide Nuclear Fuel

**Alternative Fuels I**
***Hilton San Francisco, Continental 2***
• Esterification and Transesterification of Acid Oils for Biodiesel Production Using Heterogeneous Catalyst
• Pretreatment Kinetic Characterization of Timber Varieties and Switchgrass Using Diluted Acid Hydrolysis
• Evaluation of Tall Oil as a Feedstock for the Production of Biodiesel
• *in-Situ* Transesterification of Soybeans
• Advances in Base-Catalyzed Transesterification of Soybean Oil Using Nanocrystalline Oxides

**Applications of Adsorption in Energy and Fuel Cell Technology**
***Hilton San Francisco, Continental 1***
• Adsorptive Storage of Mechanical Energy (Work) for Transportation Applications
• Modeling and Simulation of Dynamic Bio-Ethanol Adsorption
• Adsorption Separation of Methane and Carbon Dioxide from Landfill Gas
• Development of Rapid-Cycle Hydrogen PSA to Purify Catalytic Partial Oxidation (CPO) Syngas
• Room Temperature $CO_2$ Removal over $K_2CO_3$ on Porous Microfibrous Media
• Combined Hydrogen Production and Storage Via Reactive Ball Milling: Investigation of Carbon Structure for Hydrogen Capture
• Integration Study of Adsorption/Bio-Regeneration of Adsorbents for Ultra-Deep Desulfurization

**Best Practices in Electronic Structure Calculations**
***Hilton San Francisco, Imperial B***
• Density Functional Calculations
• First-Principles Calculations and Multi-Scale Modeling of Supported Nanocatalysts
• New Density Functionals Applied to Old Problems
• Elucidation of Structure-Reactivity Relationships Using Quantum Chemistry
• Simulating Fluid Phase Equilibria and Aggregation from First Principles

### Biomems and Microfluidics - Novel Applications
***Marriott San Francisco, Yerba Buena Ballroom 3***

- Rapid Prototyping of a Continuous-Flow Pcr Microchip
- Gel-Preloaded Microchips for DNA Analysis
- High-Throughput and Real-Time Study of Single Cell Electroporation Using Microfluidics: Effects of Medium Osmolarity
- A Fractal Analysis of Pathogen Detection by Biosensors
- Rapid Chip-Scale Detection by Micro-Spiral Flow and Surface Enhanced Raman Scattering
- Cell Encapsulation Using Microfluidic Device

### Cardiovascular and Cancer (I)
***Hilton San Francisco, Yosemite A***

- Modeling Delivery of Supplemental Nitric Oxide in Resistance Vessels
- A Novel, Quantifiable Three-Dimensional Model of Melanoma Invasion
- Parsing the Crosstalk between Prominent Oncogenic Signaling Pathways
- Mitochondria Depolarizing Peptides Sensitize Prostate Cancer Cells to Death Receptor Mediated Apoptosis
- Fibrin-Cd44v Binding Interferes with Platelet-Colon Carcinoma Cell Adhesion under High Shear Conditions
- Ultrasound-Enhanced Chemotherapy and Gene Delivery for Gliosarcoma Cells
- TNF-α Based Accentuation of Cryoinjury for the Treatment of Prostate Cancer-Dose, Delivery and Response

### Catalytic Hydrogen Generation - General I
***Hilton San Francisco, Continental 3***

- Mechanistic Interpretations in Methane Activation and Chemical Conversion Catalyzed by Supported Metal Clusters
- Reforming of Oxygenates for $H_2$ Production: Reactivity of Ethylene Glycol and Ethanol on 3d-Pt(111) Bimetallic Surfaces
- Hybrid Theoretical/Experimental Studies Aimed at the Development of Carbon-Tolerant Reforming Alloy Catalysts
- A Computational Study of $Fe_3O_4$ (100) Surface Species Related to Water-Gas Shift
- Mechanism for Carbide Supported Water Gas Shift Catalysts
- Spatially-Resolved Species Profiles in Millisecond Reactors: Catalytic Partial Oxidation of Methane
- Photocatalytic Water Splitting Using Titania Nanoparticles Functionalized with High-Valent Oxomanganese Complexes

### Cell Adhesion and Migration (I)
***Hilton San Francisco, Yosemite C***

- Osteogenic Differentiation of Mc3t3-E1 Cells Regulated by Substrate Stiffness Requires Mapk Activation
- Biomimetic Microcontrolled Materials for Guiding Cell Migration
- A Model for Force Generation by Microtubule End-Binding Proteins
- Combined Effect of Brain-Derived Neurotrophic Factor and ECM-Coated Substrates on Neurite Extension and Persistence from Retinal Explants
- Early Growth Phase Adhesion of *S. Aureus* to Immobilized Platelets Via Clumping Factor A (ClfA) and Fibronectin Binding Proteins (Fnbps)
- Amyloid-Beta Induced Endothelial-Monocyte Interactions Involved in Cerebral Amyloid Angiopathy and Alzheimer's Disease
- Chemoreceptors Control Salmonella Typhimurium Motility, Accumulation, and Localization in in Vitro Tumors

### Chemical Engineering Principles for Nanotechnology
***Marriott San Francisco, Yerba Buena Ballroom 6***

- Theory and Simulation for the Advancement of Nanoscience and Technology
- Nanoporous Thin Film Technology
- Nanostructured Materials for Solar-to-Electric Energy Conversion
- The Chemistry of Single Walled Carbon Nanotubes

### Chemical Technology Start-Ups
***Hilton San Francisco, Franciscan D***

- Collaborative Research Focused on the Discovery and Development of Vascular Disrupting Agents (VDAs) for the Treatment of Cancer
- Accelerating New Drugs Identification through Multi-Centric Research and Investment: a Brazilian Biotech Case
- The Pleasure, Pain and Pitfalls of Starting a New Business
- Commercialization of Specialty Polymers: a Perspective on SBIR and Contract Research Driven Technology Transfer
- Chemical Technology Startups: Overview of Activities and Opportunities

### Computational Fluid Dynamics in Chemical Reaction Engineering
***Hilton San Francisco, Franciscan C***

- Multi-Environment Probability Density Function Method for Modeling Turbulent Combustion Using Detailed Chemistry
- Modeling Coupled Reactive Flow and Evaporation within a Multistage Reactor
- Comparison of a Fully Coupled and a Decoupled Solver for the Simulation of Fluid Catalytic Cracking
- CFD Modeling of a Fixed Bed Reactor for Strongly Endothermic Reactions
- Pore-Scale Simulation of Transport Processes in Fixed-Beds: Combining a Lattice Boltzmann CFD Method and a Particle Tracking Method
- CFD Modeling of Slurry Bubble Column Reactor for Fisher-Tropsch Synthesis
- Predicting Combustion in Packed Bed Reactor Using UDFS and Eulerian Model

### Crossing Traditional Boundaries with Information Technology
***Hilton San Francisco, Lombard***

- Plant Operation Data Mining for Cost Model Enhancement
- Using Simulation-Based Optimization Approach for Space Missions' Process Synthesis and Design
- Analytical Service Laboratory Pilot Application
- Integration of the R&D Enterprise
- Roundtable Discussion: Crossing Traditional Boundaries with Information Technology

### Distillation Honors: Zarko Olujic II
***Hilton San Francisco, Mason***

- Evaluation of Higee for Distillation
- Modeling of Reactive Dividing Wall Columns
- Hybrid Membrane-Distillation Processes
- An Overview of a Japanese National Project: Development of Technology for Energy-Saving Distillation through Internal Heat Exchange (HIDIC)
- Liquid Flow Distribution in Catalytic Distillation Columns: Use of High Energy X-Ray Tomography
- Effective Mass Transfer Areas in Packed Absorbers

### Free Forum on Engineering Education I
***Hilton San Francisco, Van Ness***

- Incorporating Six Sigma Methodology Training into Chemical Engineering Education
- Integrating Computational Fluid Dynamics into the Engineering Curriculum: Demonstration Though Case Studies
- Purewaterlab: an Interactive Simulator for Promoting Water Conservation and Sustainability in Engineering Education
- Interpreting Student-Constructed Study Guides: a Constructivist/Constructionist Perspective
- Making CFD Popular among Undergraduate Students
- Integrating Process Simulators and Factorial Design of Experiments into Undergraduate Chemical Reactor Design Course

### Fuel Cell Technology II
***Hilton San Francisco, Continental 7***

- Novel and High Performance Electrodes with Nano-Hybrid Hydrocarbon Ionomers of PEMFC for Broad Temperature Range and Lower Humidity Condition
- Direct Methanol Fuel Cell System Performance: from Materials, Components, to System and Fuel Efficiency
- A Steady State Three-Dimensional Model for a PEMFC System to Simulate Water Transport and Performance Characteristics
- Water Management in a 25$cm^2$ PEM Fuel Cell with Electroosmotic Pumping
- Equivalent Circuit Models for Polymer Electrolyte Fuel Cell Stacks in Parallel at Operational Loads
- The Evaluation of the Feeding Effect on Liquid-Feed Dmfc Using Rigorous Dynamic Simulation
- Preparation and Characterization of Microporous Layers for Gas Diffusion Media

### Functional Nanoparticles and Nanocoatings on Particles I
***Marriott San Francisco, Yerba Buena Ballroom 4***

- Surface Initiated Polymerization on Magnetite Nanoparticles with Novel Fluorescent-Thermo Responsive Polymeric Shells for Biomedical Applications
- Surface Patterning of Microspheres Using Photodefinable Ultra-Thin Polymer Coatings
- Polymer Coatings on Particles Using Initiated Chemical Vapor Deposition
- Synthesis and Magnetic Properties of Silica-Coated Fept Nanocrystals
- Synthesis and Characterization of Environmentally Responsive Superparamagnetic Nanoparticles
- Properties of Surface-Asymmetric Metal-Decorated Micro- and Nanospheres
- Novel Synthesis of Polymer-Metal Nanocomposites

### Fundamentals of Supported Catalysis I
***Hilton San Francisco, Franciscan A***

- EXAFS Characterization of Pt/Dendrimer Nanocomposites Used for the Preparation of $Pt/A_{12}O_3$ Catalysts
- The Production of Highly Dispersed Metals Via "Strong Electrostatic Adsorption"
- Characterization and Kinetic Evaluation of Ag-Pt Bimetallic Catalysts Prepared by Electroless Deposition
- Deep Hydrogenation of Tetralin over Pt/Pd Catalysts: Influence of Fluorine and Catalyst Preparation
- Estimation of Transport and Equilibrium Parameters on Beta-Zeolites – Tracer Experiments on Packed Bed Reactor Systems
- Alumina-Titania Nanofibers Synthesis by pH Swing Method

### Innovations in Biopharmaceutical Development: Fast to Market, Short on Time I
***Hilton San Francisco, Plaza B***

- Improving Pharmaceutical Product Development and Manufacturing: Impact on Cost of Goods Sold of Pharmaceuticals and Cost of New Drug Development
- Risk Management in the Development of Novel Biomedical Devices and Vaccines
- High Throughput Cell Culture Development Using the Simcell Platform
- Rational Design of Protein Purification Processes
- A Case Study: Utilization of Antibody Purification Platforms - Impact on Timelines
- Large-Scale Pool-Less Purification
- Regulated Production of Biologically Active

Insulin from Engineered Human Skin Substitutes for Treatment of Diabetes

**Integrated Product and Process Design**
***Hilton San Francisco, Union Square 24***
• Property Based Approach for Integrated Process and Molecular Design
• Simultaneous Model-Based Process and Product Design Using Reverse Design Approach
• Combining Molecular and Chemical Process Simulation for Product Design
• Crystal Shape Enhancement: a Processing Solution to a Product Problem
• Design of Emulsified Products: Effects of Disperse Phase Rheology
• Microeconomics Helps Seeing That the "Best Product" Is Not the "Best Product"

**Interfacial and Electrochemical Phenomena in Microfluidics and MEMS Devices**
***Hilton San Francisco, Union Square 5 & 6***
• Analytical Model of Concentration Boundaries in Single Interface Isotachophoresis
• Separation by Cyclic Electric Field-Flow Fractionation
• Characterization of AC Voltammetric Reaction-Diffusion Dynamics: from Patterns to Physical Parameters
• Transport of Fluid and Current in Nanofluidic Channels: Importance of the Electrical Double Layer Thickness
• Microchip Based Hydraulic Pumps for Performing Pressure-Driven Separations
• Rapid Exploration of Phase Behavior in Surfactant Systems Using Microfluidics
• Spot Welding Though a Molecular Boundary Layer Due to Repetitive Contact

**Materials Engineering and Sciences Division Plenary Session**
***Hilton San Francisco, Imperial A***
• Using Molecular Design Concepts and Light to Engineer Surface Properties
• Blood-Material Interactions of Polyurethanes
• Polymer Nanogels and Networks for Bioanalytical Devices
• Experimental Diagnostics and Modeling of Microplasma Discharges
• Functional Magnetic Nanoclusters for Chemical, Biological, Medical and Environmental Applications

**Mesoscale and Nanoscale Thermodynamics I**
***Hilton San Francisco, Union Square 22***
• Freezing and Melting of Water in MCM-41 and SBA-15 Silica Materials
• Generalization of Kelvin's Equation for Compressible Liquids in Nano-Confinement
• Determination of Wetting Transitions in Binary Mixtures at Three-Phase Coexistence Using Transition-Matrix Monte Carlo and Finite-Size Scaling
• Does Confining the Equilibrium Hard-Sphere Fluid between Hard Walls Change Its Average Properties?
• Phase Behavior in Nanosystems: the Difference between the Canonical and Grand Canonical Ensembles
• Nucleation and Growth of Aluminum Nanoparticles Using Monte Carlo Simulations
• Molecular Simulation of the Self-Assembly of Bent-Core Molecules at Water Surfaces

**Microfluidics and Small-Scale Flows II**
***Hilton San Francisco, Union Square 15 & 16***
• Multiphase Microfluidic Fabrication for Biomedical Diagnostics and Regenerative Medicine
• Universality in the Size and Spacing of Slugs Generated by Converging Immiscible Flows at Microfluidic Junctions
• Numerical Simulation of Droplet Formation in Flow Focusing Microfluidics Device
• Effects of Geometry and Fluid Elasticity during Polymeric Droplet Pinch-off in Microfluidic Environments
• Dynamics of Drop Formation in Microchannels: Polymeric Fluids, Micellar Solutions, & Tip-Streaming
• Transport and Dispersion in Segmented Gas-Liquid Flow through a Forest of Micropillars
• Multilayer Microfluidic Flows of Suspensions
• Separation of Suspended Particles by Asymmetric Arrays of Obstacles in Microfluidic Devices
• Nanotextured Surfaces for the Sensing and Manipulation of Colloidal Scale Objects in Microscale Flow
• Retention of Polymer Molecules in a Cavity: a Lattice Boltzmann Study

**Microreactors: Applications for Chemical Production**
***Hilton San Francisco, Union Square 23***
• Production-Related Issues in Microreaction Technology
• Catalyst Trap Microreactor for Hydrogenation of a Pharmaceutical Intermediate
• Nonisothertmal Design of Fluid Segments for Precise Temperature Control in Microreactors
• A Micro-Structured 5 KW Complete Fuel Processor for Iso-Octane as Hydrogen Supply System for Mobile Auxiliary Power Units
• Reaction Optimization in a Microreactor Using Real-Time Analysis
• Residence Time Distribution in a Packed Bed Microreactor
• Continuous Reactions with the Micro-Enzyme-Membrane Reactor

**Molecular Assemblies in Solution: from Fundamentals to Applications (AIChE-SCEJ Joined Session)**
***Hilton San Francisco, Union Square 19 & 20***

**Plenary Session I: Water Resource Conservation, Purification, Reclamation and Reuse**
***Hilton San Francisco, Grand Ballroom A***
• The Global Challenge for Adequate and Clean Water
• Competent, Sustainable, and Cost Effective Integrated Infrastructures for Water Supply and Energy Recovery Via Strategic Design and Deployment of Advanced Technologies
• Integrated Hydrologic Science and Environmental Engineering Observatories: Their Promise and Current Status

**Plenary Session III on Membranes and Bioseparations Honoring Professor Ed Lightfoot**
***Hilton San Francisco, Continental 5***
• Production of Porous Materials by "Reactive Gelation"
• Protein Chromatography
• Metal-Affinity Separations of Nucleic Acids
• Prediction of Protein Affinity and Displacer Selectivity in Chromatographic Systems Using Multi-Scale Modeling Techniques
• Nonlinear and Preparative Chromatography

**Population Balance Modeling for Particle Formation Processes I: Nucleation, Aggregation and Breakage Kernels**
***Hilton San Francisco, Union Square 14***
• A Mechanistic Kernel for the Aggregation Phenomenon in Population Balance Models of Granulation Processes
• Evolution of Particle Size Distribution for Yeast Flocculation by Polymer Bridging: Experiment and Modeling
• Non-Quasi-Steady Single Particle Rate Laws (Evaporation or Growth) and Population Balance Simulation Methods
• Fluctuations in Solutions to the Fragmentation Equation
• Dynamic Evolution of Multi-Variate Particle Size Distributions in Particulate Processes: a Population Balance Perspective
• FCMOM: Moments and Moving Boundaries for an Accurate and Convergent PSD Reconstruction

**Process Control Applications I**
***Hilton San Francisco, Taylor***
• An Operability-Based Methodology for the Feasible Output Ranges in the Control of Non-Square Systems
• Evaluating Robustness of Embedded Model Predictive Control Using Monte Carlo Simulation
• Towards Robust Integration of Process Control and Optimization: a Chance-Constrained Approach
• Stiction Compensation in Process Control Loops
• Model Based Control of Wastewater Neutralization
• Application of a Model Predictive Control Strategy on a Fluid Catalytic Cracking Pilot Plant
• Multivariable Model Predictive Control Implementation in an Amine Unit at a Syngas (Hydrogen + Co) Plant

**Recent Advances in Molecular Simulation Methods**
***Hilton San Francisco, Union Square 1 & 2***
• Path Sampling Based Coupling of Fast and Slow Dynamical Modes in Biomolecular Reactions: Implications for Enzyme Catalysis and Implications for Mixed Quantum Mechanics Molecular Mechanics Simulations
• Modeling Large-Scale Protein Conformational Changes with the Elastic Network Model: an Approach Based on the Empirical Valence Bond Theory
• Combining Multilevel Methods with Modern Sampling Schemes
• Improved Density of States Monte-Carlo Method Based on Recycling of Rejected States
• Monte Carlo Simulation Using Reversible Mapping between Local Energy Minima
• A Generalized Hamiltonian-Based Algorithm for Rigorous Nonequilibrium Molecular Dynamics Simulation in the NVT Ensemble
• Sequential Updating Algorithms for Grand Canonical Monte Carlo Simulations
• Ensemble Optimization Based on a Rigorous Overlap Function
• Obtaining Reaction Coordinates by Likelihood Maximization

**Structure and Properties of Polymers I: Polymer Blends**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Influence of Interfacial Tension on the Morphology of Polymer Blends
• Rheology of Immiscible Polymer Blends Containing Compatibilizer
• Shear-Induced Phase Transitions in Ternary Polymer Blends
• Crystallizable Ionic Polymer - Ionic Oligomer Blends: Coassembled Nanoscale Structure and Enhanced Properties
• Blend Miscibility of Sulfonated Polystyrene Ionomer Systems
• Decoupling the Mechanical and Electrical Properties of Polymer Electrolytes
• Near Net-Shape Manufacturing of Solid-State Polymer Blends

**Supercooled Liquids and Glasses**
***Hilton San Francisco, Union Square 3 & 4***
• Robust Links between Structure / Thermodynamics and Dynamics of Supercooled Liquids
• Common Origin of Thermo-Mechanical Anomalies in Different Network Glasses
• Spatially Heterogeneous Dynamics and String-like Motion in Granular Matter and Comparison with Glass-Forming Liquids
• Novel Computational Probes of Diffusion in Supercooled Liquids and Their Application to Rotation-Translation Decoupling in O-Terphenyl
• A Parametric Equation of State near the Liquid-Liquid Critical Point in Supercooled Water
• A Stochastic Model for Describing Glassy Materials Subjected to Complex Thermal and Loading Histories
• Extension of Glass Transition Model to Mixtures

• Plastic Deformation in Amorphous Polymers : a Free Energy Landscape Approach

**Sustainable Fuels**
***Hilton San Francisco, Continental 6***
• Operation Optimization of the Lipase-Catalyzed Biodiesel Production
• Evaluation of Catalytic Activity of Anion-Exchange Resin for Biodiesel Fuel Production
• Thermodynamic Investigation of Selected Production Processes of Hydrogen from Biomass
• Tri-Glyceride Production from Algae Grown on Dairy Anaerobic Digester Effluent
• The Study on Liquefaction Residues of Wood Powder
• Microalgal Oil Extraction and *in-Situ* Transesterification
• Development of Local Biomass-Based Fuel Systems in Mekong Delta Area
• Optimal Path Synthesis under Uncertainty for Lignocellulosic Biomass to Ethanol Process Design

**Therapeutic Devices, Nanotechnology and Molecular Imprinting**
***Hilton San Francisco, Continental 4***
• Selective Recognition of Angiotensin II
• Molecularly Imprinted Polymers for the Recognition of Proteins
• Interfacial Molecular Imprinting for the Production of Immunoarrays
• Preparation of Biomolecule-Responsive Gels by Biomolecular Imprinting
• Therapeutic Contact Lenses Via Biomimetic Imprinting
• Star Shaped Molecularly Imprinted Polymer Working as a Drug Carrier
• Synthesis and Characterization of Moiety Imprinted Polymers (MOIPS) for Application in Drug Delivery

**Thin Films and Coatings Using Near and Supercritical Fluids**
***Hilton San Francisco, Union Square 25***
• Deposition of Metal Nanoparticles into Wide Area Thin Films and Ordered Arrays Using CO2-Expanded Liquids
• Covalent Molecular Assembly in Supercritical Carbon Dioxide: a Comparative Study between Derivatized Surfaces
• Critical Micelle Temperatures and Pressures for Polystyrene-Block-Polydiene in Subcritical and Supercritical Propane
• Wetting Phenomena at the $CO_2$/Water/Glass Interface
• Processing of Polymer Films under Supercritical Carbon Dioxide Studied Using a Quartz Crystal Microbalance
• Development of a Novel Microcellular Injection Molding Equipment with Supercritical Fluid and Primary Experimental Study

**Transport Processes in Nanoscale Systems I**
***Hilton San Francisco, Union Square 21***
• Axial Diffusion of Simple Gases in Nanochannels
• Lateral Diffusion in Raft-Forming Lipid Membranes on the Nanoscale
• Evaporation of Pure and Mixed Nano-Droplets: Molecular Dynamics Simulations
• First Passage Time Analysis of Diffusion through Nanopores
• Anomalous Diffusion in Molecularly Sized Nanopores
• Ionic Current Conduction in Nanometer Pores in the Presence of Single-Stranded DNA and the Role of Couterion-DNA Association

**Young Faculty in Catalysis and Reaction Engineering: Trends and Visions in Research and Education**
***Hilton San Francisco, Franciscan B***
• Leaving a Lasting Impression: Ideas for Attracting and Inspiring Future Chemical Engineers
• A 'Reactive Process Engineering' Course
• Chemical Reaction Engineering - Fuel for Thought
• Reaction Engineering and Catalysis for Life Science Applications
• Nanostructured Catalytic Materials for Chemical Sensors
• Ignition of Catalytic Partial Oxidation on Platinum and Rhodium Catalysts
• Environmental Applications of Computational Chemistry
• Kinetics of Elementary Arsenic and Selenium Reactions

**WEDNESDAY, 15 NOVEMBER 2006**
***11:15 AM - 12:15 PM***
**58th AIChE Institute Lecture**
***Hilton San Francisco, Grand Ballroom A***
• Thermodynamic and Kinetic Origins of Alzheimer's and Related Diseases: a Chemical Engineer's Perspective

**WEDNESDAY, 15 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**(22b) Nanomagnetics for Bioseparation**
***Hilton San Francisco, Sutter***
• Synthesis and Steric Stabilization of Magnetite Nanoparticles with Triblock Copolymers
• Air-Stable Highly Magnetic FCC-Cobalt Nanoparticles
• Biocompatible and Biodegradable Nanoparticle Labels
• Overview of the European Research Program Nanobiomag
• Is It Del B, or Del B^2? That Is the Question

**(22b) Nanoscale Science and Engineering in Biomolecular Catalysis II**
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Encapsulation of Sole Protein as Biocatalytic Nanogels
• A Biomimetic Liquid Membrane Containing a Surfactant-Coated Biocatalysis for Chiral Separation
• Enhanced Stability of Enzymes Adsorbed Onto Nanoparticles
• Biomolecules-Assisted Dispersion of Carbon Nanotubes
• Various Biocatalytic Enzyme-Nanofiber Composites
• Cellulase Activity on Thin Films of Cellulose by QCM and Spr

**Advanced Computations for Environmental Applications I**
***Hilton San Francisco, Union Square 19 & 20***
• Quantitative Structure Biodegradation Relationships for Organic Pollutants in Water and Soil
• Cluster Analysis to Investigate Air Quality Trends in Houston, Tx
• Computation of Equilibrium States in Food Networks Using Interval Analysis
• A Robust Measure of Food Web Intervality and the Dimension of Niche Space
• Stochastic Modeling of Bacterial Migration in Porous Media
• Bayesian Formulation for Predicting Fecal Coliform Bacteria Count in Mobile Bay

**Advances in Distillation Modeling and Processes II**
***Hilton San Francisco, Mason***
• Modeling and Process Design of an Internally Heat-Integrated Distillation Column
• The Automated Generation of Constrained Models from Feasibility Analysis for Reactive Distillation
• Reactive Distillation: Analysis of the Topology of a Reactive Residue Curve Map for a Continuous Column
• Process Analysis of Membrane Assisted Reactive Distillation
• Analysis of Absorption with Complex Reaction Kinetics
• Ratesep - a New and Innovative Rate-Based Distillation Model for Amine Acid Gas Treating Processes

**Alternative Fuels II**
***Hilton San Francisco, Continental 2***
• Comparative Studies on the Production of Biodiesel and the Analysis of Its Properties and Potential from Pongamia and Waste Cooking Oil
• Production of Biodiesel from Peanut Oil by Transesterification
• Emissions from Hydrogen-Compressed Natural Gas Fueled Vehicles Involving Various Driving Cycles
• Stable Oxides on Chars and Impact of Reactor Materials at High Temperatures
• Fischer-Tropsch Synthesis in Microstructured Reactors: from Laboratory to Commercial Systems

**Applications of Environmental Catalysis I**
***Hilton San Francisco, Union Square 17 & 18***
• Advanced Oxidation Processes for the Destruction of Chlorinated Pesticides: Free Radical Mechanisms, Pathways, Products and Reaction Products
• Dechlorination of Polychlorinated Biphenyls in Sediment Slurries by Palladium Modified Zerovalent Iron
• Integrated Reductive/Oxidative Treatment of Nitroaromatic Contaminated Groundwater
• Oscillating Magnetic Field Gradient Induced Motion of a Magnetic Photocatalyst
• Catalytic Oxidation of Total Reduced Sulfur Compounds from Pulp and Paper Industries with Ozone as an Oxidant
• Solar Photocatalytic Treatment of Atrazine-Contaminated Agricultural Water in the Rio Grande Basin
• The Effect of Nanostructured MnOx Crystallographic Phase and Particle Size in the Catalytic Decomposition of Hydrogen Peroxide for Environmental Remediation of Effluents

**Biomaterials II**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Multilayer Core-Shell Nanocomposite Particles for Enhanced UVA/UVB Protection in Sunscreens Via Atomic Layer Deposition
• Strong Effects of Charge and Salt on Polymersome Membrane Elasticity
• Crosslinked, Self-Assembled Protein Nanocapsules
• Design of Nanoparticle Charge and Architecture for Modulation of Cell-LDL Interactions Underlying Atherogenesis
• Asymmetric $CaCo_3$ Crystal Growth through Confinement
• Gramicidin Channel Incorporated Bilayer Supported on Hierarchical Porous Inorganic Membrane
• Nonfouling and Responsive Zwitterionic Hydrogels with Improved Mechanical Properties

**Biosensors**
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Immobilization of Myoglobin from Horse Skeletal Muscle and Hemoglobin I from Lucina Pectinata in Hydrophilic Polymer Networks for Hydrogen Sulfide Biosensor Application
• Atomic Force Microscopy Investigation of Spacer Length Effect on *Escherichia Coli* Pili-Antibody Molecular Recognition
• Simultaneous Detection of Botulinum Neurotoxins in Buffer and Honey Using a Surface Plasmon Resonance Sensor
• Biosensor Incorporating Cell Barrier Architectures for Detecting Staphylococcus Aureus Alpha Toxin
• Biosensor for Real-Time Label-Free Detection of Staphylococcal Enterotoxin B
• Layer-by-Layer Electrostatic Assembly of Carbon Nanotube Based Glucose Sensors
• Modeling Oxygen Transport and Fluid Flow within a Three-Dimensional Tissue Engineering Perfusion Bioreactor Using Finite Element Methods

**Biosensors and Tissue Engineering**
***Hilton San Francisco, Continental 4***
• Effect of Electrode Modification by Polyion Adsorption on Electrochemiluminescence of Luminol
• Construction of Mercapto-Ended Poly(Ethylene Glycol) Tethered Chain Surface for High Performance Bioconjugation
• Low Melting Point Agarose Gel as a Protection Layer in the Preparation of Aligned Binary Protein Patterns by Photolithography
• Precise Tissue Assembly Using Avidin-Biotin Binding System and Optical Tweezers
• Regenerative Artificial Vascular Graft Using Acellular Scaffold
• Construction of Nephron by Fusion of Adult Glomeruli to Ureteric Buds with Type V Collagen
• Synthesis and Characterization of Hydrogels Grown on Surfaces by ATRP
• Cell Growth on Biodegradable Poly(Depsipeptide-Co-Lactide) Matrix Releasing Growth Factors as Scaffold for Tissue Engineering
• Antiwearable and Biocompatible Surface of Artificial Hip Joints by Nano-Scaled Grafting with Phospholipid Polymers

**By Invitation: FPBE Division Plenary Lectures**
***Hilton San Francisco, Imperial A***
• Recent Advances in Cancer Treatment and Detection Using Nanoparticle Systems
• Characterization and Regulation of Hematopoietic Stem Cell Differentiation in Culture
• Biofunctional Nanoparticles
• Introduction of Prof. James Liao
• Systems Biology: a Fusion between Biology and Engineering

**Carol in Thermoland I: a Session in Honor of Carol Hall's 60th Birthday**
***Hilton San Francisco, Imperial B***
• What Happened to the Work with Carol
• "Singular Diameters" and the Nature of Order Parameter in Asymmetric near-Critical Liquid Mixtures
• Connectedness in Irreversibly Built Structures
• Computational Nanoscience
• Effects of Confinement on Freezing and Melting

**Catalytic Hydrogen Generation - General II**
***Hilton San Francisco, Continental 3***
• Kinetic Study of Ammonia Decomposition on Tungsten Carbide for Cleaner Production of Hydrogen from Biomass Gasification
• Aqueous Phase Reforming of Bio-Derived Organic Compounds
• Aqueous-Phase Reforming of Ethylene Glycol with Supported Pt and Pd Bimetallic Catalysts
• Modified Ferrite Based Catalysts for Ultra-High Temperature Water Gas Shift Reaction for Membrane Reactor Applications
• Precious Metal Monolithic Catalysts for Fuel Processing – Overcoming the Limitations of Base Metal Particulate Catalysts
• Development of a Combined Catalyst and Sorbent for Hydrogen Production
• Improvement of Methane Steam Reforming by Using Equilibrium Shift with Lithium Silicate

**Characterization of Nanoporous Materials**
***Hilton San Francisco, Powell***
• Applicability of the B.E.T Method for Obtaining Surface Areas in Metal-Organic Frameworks
• Understanding the Mechanical Properties of Nanoporous Au
• Evaluation of Thermoporometry for the Characterization of Mesoporous Materials
• Microstructural Analysis and Adsorption Properties of Porous Carbons Using Molecular Simulation
• Characterization of Cubic Mesoporous Tio2 Thin Films by Spectroscopic Ellipsometric Porosimetry Technique
• Three-Dimensional Reconstruction of Mesoporous Materials Using Gas Adsorption and Structure Factor Data
• Structural Characterization of SBA-15 Silica by 29SiB-NMR and *in-Situ* Synchrotron Small-Angle Diffraction Studies of Physisorbed Films
• Characterization of Polymer-Templated Micro-Mesoporous Silicas by Gas Adsorption, Small Angle X-Ray Scattering and DFT Modeling

**Complex Multiphase Flows**
***Hilton San Francisco, Union Square 22***
• Direct Numerical Simulation of Reactive Deformable Bubble Swarms in Non-Newtonian Fluids
• Rheology of Fluids with Monodisperse Microbubble Suspension
• Non-Brownian Microrheology of a Fluid-Gel Interface
• Dynamic Interfacial Tensiometry
• Sedimentation of Flexible Fibers with Inertia
• Simulation of Rodlike Particles in Field-Flow Fractionation (F.F.F.)
• Rheological Measurements on Extremely Concentrated Suspensions Using Squeeze Flow
• Rheology and Mesoscale Network Structure of Entangled Polystyrene-Organoclay Solutions
• Rheological Behavior of Polymer Melts in Equibiaxial Elongational Flow Using a Modified Lubricated Squeezing Flow Technique
• An AC Electrokinetic Micropump Based on Field-Induced Secondary Maxwell and Back Pressure Gradients along a Continuous Wire Loop

**Computational Modeling of Surfaces and Surface Phenomena**
***Hilton San Francisco, Union Square 1 & 2***
• Chiral Adsorption on Cu Surfaces
• Development of the Oxygen Reduction Reaction Mechanism on Pt(111) Using DFT
• The Growth of Thin Metal Films on Polar Metal Oxides Surfaces: Insights from First-Principles Calculations
• Strong Repulsive Forces between Protein and Phosphocholine Self-Assembled Monolayers - a Molecular Simulation Study
• Effects of the Combined Action of Electric Fields and Mechanical Stresses on the Morphological Stability of Solid Surfaces
• Ab Initio Phase Diagrams for Water Adsorbed on Monoclinic $HFO_2$
• Molecular Simulation Study of Nanoscale Friction between Phosphocholine Self-Assembled Monolayer Surfaces Immersed in Ionic Solution

**Diffusion in Polymers I**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Diffusion Enhancements in Mineral Nanoparticle Filled Superglassy Polymers
• Reverse Selectivity in Poly Dimethyl Siloxane/Au Nanocomposite Membrane in $CO_2/Ch_4$ Separation
• Modeling of Enhanced Penetrant Diffusion in Nanoparticle-Polymer Composite Membranes
• Penetrant Transport in Well-Characterized Glassy Polymers as Revealed by High-Resolution X-Ray Computed Tomography
• Modeling Sorption Kinetics of Carbon Dioxide in Initially Glassy Polymers Using Non-Equilibrium Thermodynamics
• Fundamental Diffusion Behavior of Polymer Ultrathin Films: Effect of Film Thickness, Molecular Weight, and Aging
• Role of the Diffusion in the Transport of Gas Species through Polymer Membranes

**Dynamics and Modeling of Particulate Systems I**
***Hilton San Francisco, Franciscan D***
• Numerical Simulation of Liquid Transfer between Particles
• Tomographic Imaging of Electrostatic Charges and Charging Phenomena in Particulate Flow Systems
• Modeling of Granular Mixing Using a DEM-Based Markov Process Method
• Experimentally Validated Computations of Heat Transfer in Granular Flow in Rotary Calciners
• Characterization of Granular Mixtures by Comparison to Chemical Solution Theory
• Knudsen Boundary Layer in Granular Systems
• Clustering of Sand Grains Due to Triboelectrification

**Emerging Cyber Infrastructure Trends and Capabilities**
***Hilton San Francisco, Lombard***
• A Cyber-Infrastructure for Catalysis Science
• The Infrastructure in Cyberinfrastructure: Observations of Large Scale Investments in Asia
• A Multidisciplinary Cyberinfrastructure Approach
• Opportunities for Cyberinfrastructure Funding in NSF's Engineering Directorate
• Collaboration Technologies in Engineering and Science
• Panel Discussion on Emerging Cyberinfrastructure

**Environmental Effects of Nanotechnology and Nanomaterials**
***Hilton San Francisco, Union Square 15 & 16***
• Deposition of Nanoparticles in the Human Respiratory Tract
• Sol-Gel Synthesis of Nanocrystalline Oxide Adsorbents for the Adsorption of Thiophene from Hydrocarbon Liquid
• Comparative Solubility of Nanoparticles and Bulk Oxides of Magnesium in Water and Lung Simulant Fluids
• Towards a Systems View in Nanotechnology- Life Cycle Assessment of Nanoparticles Synthesis
• Nanostructured Materials as Smoke Clearing Agents
• A Review of the Toxicity of 0.1 to 1 Micron Aerodynamic Diameter Airborne Particles
• Nanometallic Fuels for Transportation: a Well-to-Wheel Analysis

**Flow Visualization and Tomography**
***Hilton San Francisco, Franciscan C***
• Genetic Algorithm Based Fast X-Ray Ct Technique Applied in Multiphase Flow Measurement
• Simulation and Experimental Studies in Dual Source Gamma Ray Computer Tomography for Imaging Three Phase Systems
• Imaging Large Vessels Using Cosmic-Ray Muon Energy-Loss Techniques
• Linking 3-D Electrical Tomography Imaging to Fluid Flow Patterns in an Annular Flow Fixed-Bed Reactor

**Free Forum on Engineering Education II**
***Hilton San Francisco, Van Ness***
• Pedagogical and Learning Advantages Realizable through Scaling and Non-Dimensionalization
• Forget about Teaching: It Is All about Learning!
• Using Inquiry-Based Activities to Promote Understanding of Critical Engineering Concepts
• The Effect of Cooperative Learning Experiences and Instructional Methods on Chemical Engineering Students' Self-Efficacy Beliefs
• A Multidisciplinary Undergraduate Research and Development Program to Enhance Education and Diversity in Science and Engineering
• Using Personal Response Devices in the Classroom

**Fuel Cell Portable Power Systems I**
***Hilton San Francisco, Continental 8***
• Silicon Microreformer for the Evaluation of Thermal Integration Issues in Microscale Fuel Processing
• Design and Integration of Portable SOFC Generators
• Micro-Structured Reactor Technology for Portable Fuel Processors
• Current Status of Silicon Based Micro Fuel Cells for Portable Power
• Portable Power through Liquid Fuel Reforming in Microchannel Reactors

• Air-Breathing Multi-Channel Laminar Flow Fuel Cells

**Functional Nanoparticles and Nanocoatings on Particles II**
***Hilton San Francisco, Union Square 14***
• Preparation of Nano-Gypsum from Anhydrite Nanoparticles: Strongly Increased Vickers Hardness and Formation of Calcium Sulfate Nano-Needles
• Shape Control of Electrostatically Capped Platinum Nanoparticles without Aid of Foreign Metal Ions
• Functionalization of Composite $Al_2O_3$/Metal Varistors Based on ALD Surface Modified Particles
• Synthesis of Uniformly-Sized High Quality CdSe Tetrapods in High Yield
• Passivation of SiB Nanocrystals Using Photo-Assisted Alkylation
• Simultaneous Nanoparticle Formation and Attachment to the Surface of Glass Beads by Plasma Enhanced Chemical Vapor Deposition
• Electrostatic Self-Assembly of Binary Nanocrystals with a Diamond-like Lattice

**Fundamentals of Supported Catalysis II**
***Hilton San Francisco, Franciscan A***
• Identification of Reaction Sites on Supported Metal Catalysts
• Structural Changes in Au Nanoparticles and in $Tio_2$ during the Oxidation of $CH_4$ and $C_2H_4$ on $Au/TiO_2$ Catalysts
• In Situ Modification of a Pt Catalyst Supported on a Mixed Ionic-Electronic Conducting Membrane
• Structure and Reactivity of Model Supported Pd-Zn Bimetallic Methanol Steam Reforming Catalysts
• Sintering Studies on Model Catalytic Systems
• Kinetics of Nh Formation and Dissociation on Pt(111)

**Hydrogen Production Process Design and Economics**
***Hilton San Francisco, Union Square 13***
• Consistent Economic Analysis of Hydrogen Production Pathways
• Plant Design and Cost Analysis of a Prototype Commercial Nuclear Hydrogen Production Plant
• First Order Approximation of Hydrogen Delivery System Costs
• Innovative Nuclear Process Heat Applications for near-Term Hydrogen Production
• A Low-Greenhouse-Impact Hydrogen-Based Liquid-Fuels Future
• Economic Implications of Peak Vs. Base Load Electricity Costs on Nuclear Hydrogen Systems

**Innovations & Opportunities in Biopharmaceutical Development-Invited Papers**
***Hilton San Francisco, Yosemite C***
• Biopharmaceutical Development Opening Remarks
• High-Throughput Biocatalysis for Drug Discovery and Development
• Adsorptive Separations of Proteins and Nucleic Acids: Macro, Micro and Nano
• pH-Triggered Liposomes for RNAI Delivery
• "Body-on-a-Chip" Technology for Predicting Human Response to Various Drug Therapies
• Development Challenges & Opportunities
• Innovations in Biotechnology Panel Discussion

**Innovations in Biopharmaceutical Development: Fast to Market, Short on Time II**
***Hilton San Francisco, Plaza B***
• Think out of the Box - a Case Study of a Photosensitivity Phenomenon during Mab Product Recovery
• Targeting Lentivectors to CD34+ Hematopoeitic Stem Cells for Gene Therapy
• Degradable Nanoparticles as Efficient and Versatile Nonviral Gene Carriers
• Electrosonic MEMS Gun for Efficient Cellular Transfection and Drug Delivery
• Using Light Illumination to Control DNA Condensation
• Approaches to Efficient Pre-Clinical Process Development
• Detection of Protease Activity in Hydrolysates Additives: Effects on Monclonal Antibody Product Quality and Downstream Purification

**Interfacial Phenomena in Materials Processing / Composites**
***Hilton San Francisco, Union Square 5 & 6***
• Interfacial Stress Transfer in Carbon Nanotube Systems
• Substrate Effects on Polymer Thin Films as an Analogy for Polymer Nanocomposites
• Effect of Counter-Ion Concentration on the Rheology of Shear-Thickening Surfactant Solutions
• Responsive Binders for Controlling Dispersion Behavior of Fine Particle Clusters
• Reversible Aggregation of Nanoparticles Induced by pH Dependent Changes of a Self-Assembled Polypeptide
• pH-Induced Dispersion of Nanoparticle Clusters
• Single-Step Synthesis of Metal/Porous Support Nanocomposite Materials in Mixed Surfactant Mesophase

**Modeling Transport through Membranes**
***Hilton San Francisco, Yosemite A***
• Design of Novel Porous Membranes for High Efficient $CO_2/N_2$ Separation Using Combinatorial Simulation Technique
• Diffusion through Membranes from Spatially Distributed Sources
• Effects of Morphological Properties on the Permeability of Reconstructed Porous Media
• Molecular Simulations of Pervaporation Separations Using Zeolite Membranes
• Experimental and Model Description of Combined Effects between Stress and Diffusion in Glassy Polymers
• Permeability of H in Pd-Based Alloys Using Density Functional Theory
• Predicting Hydrogen Permeance in Composite Pd-Porous Support Membranes

**Molecular Modeling in Electronic Materials Processing**
***Hilton San Francisco, Union Square 25***
• Mechanisms for Interstitial-Mediated Transient Enhanced Diffusion of Arsenic and Phosphorus Dopants
• An Investigation into Gallium Arsenide Thin Film Growth: Molecular Dynamics Simulation
• Ab Initio Simulations of Surface Chemistry for Thin Film Growth of Electronic Materials
• A Computational Microscopy Study of Self-Interstitial Aggregation in Ion-Irradiated Silicon
• Analysis of Misfit Dislocation Formation and Strain Relaxation in $SiB_{1-X}Ge_X$ Thin Films on SiB (100) Substrates
• Kinetic Monte Carlo Simulations of Void Morphological Evolution in Silicon in the Presence of Oxygen

**Nano-Energetic Materials**
***Hilton San Francisco, Continental 9***
• Role of Nano-Particles in Energetic Materials Development
• Experimental and Modeling Studies of Self-Sustaining Reactions between Nanopowders
• Nanoscale Materials Environmental and Health Issues
• Solution Combustion Synthesis Boosts Ceria Activity Towards Diesel Soot Combustion

**Nanoscale Science and Engineering Award Lectures**
***Marriott San Francisco, Yerba Buena Ballroom 6***

**Novel Numerical Methods in Fluid Mechanics**
***Hilton San Francisco, Continental 1***
• Pseudospectral Simulation of Homogeneous Turbulent Shear Flow without Remeshing
• Numerical Simulation of Scalar Transport in Flows over Complex Surfaces
• Assessing the State-of-the-Art in Preconditioned Iterative Solvers for Strongly Convected, Three-Dimensional, Incompressible Flows
• Interfacial Dynamics in Stokes Flow Via a Three-Dimensional Fully-Implicit Interfacial Spectral Boundary Element Algorithm
• Accurate Continuation of Multi-Dimensional Fem Calculations Involving Drop Breakup beyond the First Singularity
• New Finite Element Formulations for Viscoelastic Fluid Flows
• Generalized Brownian Configuration Fields for Fokker-Planck Equations Including Center-of-Mass Diffusion
• An Efficient Algorithm for Multiscale Flow Simulation of Dilute Polymeric Solutions Using Bead-Spring Chains
• Ewald-like Method for 3d-Confined Systems: Electrostatics and Hydrodynamic Interactions
• Using Brownian Dynamics to Model Nanoparticle Aggregation under Shear

**Novel Polymer Product Designs and Applications**
***Hilton San Francisco, Union Square 24***
• Improved Seal Materials for Use in Food and Pharmaceutical Processes
• Formulation of Water-Soluble Polymer Coatings by Modifying Rheological Properties, Atomization, and Coating Strength of Polymer Aqueous Solutions
• Influence of Phase Segregation on the Mechanical Properties of Blends of Polyethylenes That Differ Considerably in Molecular Weight
• Erodible Multilayered Films Fabricated from Degradable Polyamines: Influence of Polymer Structure and Film Architecture on Film Erosion and Controlled Release

**Plenary Session II: Water Resource Conservation, Purification, Reclamation and Reuse**
***Hilton San Francisco, Grand Ballroom A***
• Advances in Seawater RO Desalination
• Inland Water Desalination and Reclamation - Issues and Challenges
• Industrial Experience with Water Resource Conservation, Purification, Reclamation and Reuse

**Plenary: Frontiers in Renewable Energy**
***Hilton San Francisco, Continental 6***
• Future of Solar Energy

**Polymer Thin Films and Interfaces V: Conducting Organics**
***Hilton San Francisco, Plaza A***
• Water-Dispersible, Conductive Polyaniline Makes Better Electrical Contacts to P-Type Organic Semiconductors in Otfts
• Electrochemical Devices Via Electrostatic Nanoscale Assemblies
• Small Angle Neutron Scattering Measurements of Poly(3,4-Ethylene Dioxythiophene) : Poly(Styrene Sulfonic Acid) Dispersions and Thin Films
• Donor-Acceptor Conjugated Copolymers for Ambipolar Field-Effect Transistors
• Surface Chemical Modification to Systematically Vary the Dielectric Interface in Semiconducting Polymer Field Effect Transistors

**Process Control Applications II**
***Hilton San Francisco, Taylor***
• Identification of Unmeasured Disturbances in Mpc Plant Test Data
• Soft Sensors for Quality Prediction Using Neural Networks
• Spatial Reconfiguration of Reactor Operation with Genetic Algorithms and Online Learning in Reactor Networks

• A Plantwide Control Procedure Applied to the HDA Process
• Plant Wide Reconfigurable Control in the Face of Sensor and Actuator Failures: Supervisory Architecture and Application to Tennessee Eastman Process
• Dynamic Modeling and Control of the Prico© LNG Process
• Role of Multiplicity in Control System Design for a Methyl Acetate Reactive Distillation Column

**Rational Catalyst Design I**
***Hilton San Francisco, Franciscan B***
• Ab Initio Molecular Design of Catalysts for Ethylene and Styrene Polymerization and Methane to Methanol Conversion
• First-Principles Design of Metal Alloy Catalysts for Electrocatalytic Methanol Oxidation
• Molecular Insight into Carbon Poisoning of Ni Surfaces: DFT-Guided Formulation of Carbon-Tolerant Steam Reforming Catalysts
• Fuels and Chemicals from Low-Temperature Catalytic Conversion of Glycerol to Synthesis Gas
• Design of a Stable Mononuclear Supported Gold Catalyst on Cerium Oxide: Synthesis and Spectroscopic Characterization during Carbon Monoxide Oxidation Catalysis
• An *Ab-Initio* Study of Methanol Synthesis on Cu Catalysts

**Self Assembly in Solution I**
***Hilton San Francisco, Union Square 3 & 4***
• The Role of Confinement on the Evolution of Surfactant Mesophases
• Photorheological Fluids: Micellar Systems with Viscosity Tunable by Light
• Molecular Dynamics Modeling of Reverse Micelles: Dynamics of $ZrO_2$ Particles in the Core
• A New Class of Self-Assembled Organogels Induced by Bile Salts at Submillimolar Concentrations
• Micellization of Triblock Copolymers Comprised of PEO Tail Blocks and Center Blocks Containing Carboxylic Acids
• Structural Evaluation of Gold Nanoparticles with an Ionic Organic Corona: Single Component, High Nanoparticle Volume Fraction Fluids for Enhanced Optical Properties and Processability
• Aqueous-Core Capsules Via Interfacial Free Radical Alternating Copolymerization

**Separations Design**
***Hilton San Francisco, Yosemite B***
• Synthesis of Crystallization Processes for Systems Involving Solid Solutions
• Distillation Column Systems
• A Novel Search Space Formulation for the Synthesis of Separation Networks
• An Automated Feasibility Evaluation Algorithm for Reactive Distillation
• New Design Method for Crude Fractionation
• Hybrid -Pervaporation-Distillation Processes – a Novel Heat-Integration Approach
• Multi-Objective Optimization of Hybrid Batch Distillation/Pervaporation Processes

**Separations in Biopharmaceutical Downstream Processing I**
***Hilton San Francisco, Continental 7***
• Comparison of a New Continuous Chromatographic Solvent Gradient Process for Bioseparations with Conventional Processes
• Scale down Model Demonstrates High Product Throughputs with Disposable Anion Exchange Chromatography
• Downstream Separation and Scale-up Challenges for *E.Coli*-Derived Biopharmaceuticals – an Industrial Study on Development of an Antibody Fragment (Fab) Process
• A Toolbox for Efficient Release and Recovery of Therapeutic Proteins from the Periplasm of Pseudomonas Fluorescens
• Diverse Transgenic Plant Hosts Challenge Downstream Process Development
• High Throughput Protein Purification Using Negative Mode Hydrophobic Interaction Chromatography
• Separation of Pharmaceutical Process-Related Impurities by an Organic Solvent Nanofiltration Membrane Cascade

**Structure and Properties of Polymers II: Networks and Gels**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Impact of Solvent on the Mechanical and Adhesive Properties of Solvent Swollen Polymer Gels
• Structure and Dynamics of Self-Assembled Liquid Crystalline Gels
• Enhanced Mechanical Properties of Multimodal Polydimethylsiloxane Networks
• Mechanical Properties of Highly Cross-Linked Network Polymers
• Peptide-Modified Responsive Networks with Built-in Logic
• Photoinduced Stress Relaxation and Actuation in Crosslinked Polymers
• Photoresponsive , Amphiphilic Copolymers of Azobenzene and N,*n*-Dimethylacrylamide

**Sustainable Nonfuel Products/Production Systems from Biomass Resources**
***Hilton San Francisco, Continental 5***
• α-Olefins Synthesis from Fischer-Tropsch Reaction in a Trickle Bed Reactor
• Economical Evaluation of Biomass-Fired Power Generation in Japan
• Microwave Irradiation as an Alternative Pretreatment Method for Sludge Stabilization
• Methane Fermentation of Seaweed Biomass
• Hydrothermal Pretreatment of Lignocellulosics for Ethanol Fermentation
• A Kinetic Study on Hot-Water Extraction of Woodchips
• Productions of Chitin and Valuable Substances from Crab Shell Using Sub-Critical Water

**Technology Roadmap: Pharmaceutical Product Development & Manufacturing I**
***Hilton San Francisco, California Room***
• Technology Roadmap: Context and Drivers for Roadmap Development
• Technology Roadmap: Pharmaceutical Materials Component
• Technology Roadmap: Product Development Component

**Transport Processes in Nanoscale Systems II**
***Hilton San Francisco, Union Square 21***
• Influences of Nanoscale Structural Features on Transport through Self-Assembled Monolayers
• Knudsen Diffusion in Rough Nanopores: Discussion of a Paradox
• Anisotropic Thermal Conductivity of Nanoscale Confined Thin Films Via Lattice Boltzmann Method
• Molecular Simulations of Water Transport through Single-Walled Aluminosilicate Nanotubes of Tunable Dimensions
• Molecular Sieving Using Single Wall Carbon Nanotubes
• Direct Nano-Flux and Thermomechanical Analysis of Gas Separation Nanocomposite Membranes

**University Collaboration Panel**
***Hilton San Francisco, Union Square 23***
• A Pharmaceutical Industry – University Research Collaboration Via a Post-Doctoral Researcher: the Industrial Perspective
• University and Industry Collaboration on Commodity Versus Entrepreneurial Products
• Collaboration through an NSF-Goali Project
• University of Maryland High Shear Mixing Research Program
• National Institute for Pharmaceutical Technology and Education

**WEDNESDAY, 15 NOVEMBER 2006**
***3:00 PM - 6:00 PM***
**Separations in Biopharmaceutical Downstream Processing II (Including Pat Applications)**
***Hilton San Francisco, Continental 7***
• Utilizing on-Line HPLC to Enable Process Monitoring, Automation, and Control of Downstream Unit Operations in a Biopharmaceutical Process
• Instantaneous Microbial Detector for Pat Application
• Affinity Enhanced Gel Permeation Chromatography of Proteins upon Modification with Multi-Ligand Affinity Carriers
• Purification of Factor V Leiden Molecule from Homozygous Patient's Plasma for Biosensor Development
• Preparative-Scale Dynamic Field Gradient Focusing: Proof of Concept
• Managing the Risk of Residual Moisture on Lyophilized Products from Elastomer Closures
• Manipulation of the Adsorption of Factor II, a Protein C Homologue, Using Imidazole during Immobilized Metal Affinity Chromatography Purification of Protein C from Cohn Fraction IV-1

**WEDNESDAY, 15 NOVEMBER 2006**
***3:15 PM - 5:45 PM***
**(22b) Applications of Magnetic Nanoparticles in Biotechnology and Biomedicine**
***Hilton San Francisco, Sutter***
• Magnetic Resonance Imaging Contrast Agents for Monitoring Drug Delivery *in Vivo*
• Dispersion of Super Paramagnetic Iron Oxide Nanoparticles in Poly(D,L-Lactide-Co-Glycolide) Microparticles
• Size Controlled Synthesis of $Fe_XPt_{100-X}$ Nanoparticles for Self-Regulated Magnetic Fluid Hyperthermia
• New Immunomagnetic Beads for T Cell Depletion
• Anisotropic Encapsulation of Magnetite Nanocrystals in Biphasic Nanocolloids by Electrified Co-Jetting
• Studies of Implant Assisted Magnetic Drug Targeting
• Multi-Functional Nano-Entities for Seamless Breast Cancer Detection and and Tumor Specific Treatment
• Synthesis and Characterization of Nanocomposite Hydrogels

**(22b) Bionanotechnology for Gene and Drug Delivery**
***Hilton San Francisco, Union Square 23***
• Folate Conjugated Polymer Micelles Formulated with *TPGS* for Selective Tumor Targeting
• Cationic B-Cyclodextrin Polymers for Controlled Drug Delivery across the Blood Brain Barrier (Bbb)
• Searching for Optimal Properties of Synthetic Gene Vectors Via Simulations of Intracellular Transport Processes
• Hydrodynamic Self-Assembly of DNA-Pei Nanoparticles in a Microfluidic System for Gene Delivery
• Efficient Nuclear Delivery of Antisense Oligonucleotides by Neutral, Self-Porating Polymersomes
• Core-Shell Drug Nanoparticles for Therapeutic Delivery
• Biodegradable Biphasic Nanocarriers for Multiple Drugs Delivery with Complex Release Profiles in a Controlled Manner
• Microfluidic Phase Inversion Nanoencapsulation

**(22b) Nanoscale Science and Engineering in Biomolecular Catalysis III**
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Designing Sol-Gel Materials for Biofuel Cells
• Utilization and Transport in Mediated Enzyme Electrodes with Multiscale Supports
• Applications of Biomolecular Motors in Nanotechnology

• Enzymatic Biofuel Cell Optimization and Anode Characterization
• Application of Enzyme Coated Nanofiber to Biodegradation Process
• Smart Single-Enzyme Nanogels

**Adaptive/Responsive Interfaces**
***Hilton San Francisco, Union Square 1 & 2***
• Evaluating and Improving the Stability of Organic Monolayer Coatings
• Binding and Release of Hydrophobic Analytes Using Electrically-Responsive Self-Assembled Monolayers
• Kinetics of Response for pH-Active Copolymer Thin Films
• Designed Peptide Surfactants Form a Stimuli-Responsive Film at the Fluid-Fluid Interface
• In Situ Monitoring of "Smart" Polyacrylamide Copolymer Phase Transition at the Solid-Liquid Interface
• Engineering Physico-Chemical Polyelectrolyte Multilayer Films
• Characterization of Polyelectrolyte Multilayer Films Formed at Interfaces between Thermotropic Liquid Crystals and Aqueous Phases

**Advanced Computations and Numerical Models in Water Technology and Resource Management - I**
***Hilton San Francisco, Plaza A***
• Modeling Macrotransport and Microtransport for Removal of Natural Organic Matter by Anion Exchange
• Neural Network Approach for Modeling the Performance of RO Membrane Processes
• Computational Fluid Dynamic Analysis of RO Membrane Performance with Novel Feed Spacer Geometries
• Comparative Analysis of MILP and MINLP Single Contaminant Models in the Design of Water Networks in Industrial Settings
• Mercury Trading in Water: Application of Stochastic Programming for Decision Making
• Water Height Prediction in Mobile Bay Using Wavelet-Based Multi-Scale Model

**Advanced Computations for Environmental Applications II**
***Hilton San Francisco, Union Square 19 & 20***
• Software for Modeling Multiple Emissions in a River
• Optimal Control of Lake pH for Mercury Bioaccumulation Control
• A Mechanistic Modeling Framework for Describing Tertiary Recycling of Polymers
• Effect of Acidic Sites and Calcium Hydroxide on Adsorption of Mercuric Chloride in Activated Carbon: a Molecular Simulation Study
• Odor Emission Removal from Gaseous Streams by the Use of Zeolites: a Molecular Simulation Approach
• Process Optimization for Biodiesel Production from Waste Frying Oil Using Response Surface Methodology
• The Use of the Modified Spline Method to Optimize Photochemical Reactors
• Jet Fuel Remediation at Paulinia Refinery (Replan), Sao Paulo, Brazil

**Advanced Hydrogen Storage Systems**
***Hilton San Francisco, Union Square 13***
• Hydrogen Storage in Carbon Nanotube and Palladium Composite Materials
• The Application of Steam Hydrolysis of Chemical Hydrides to Facilitate Hydrogen Storage and Generation
• Modeling Hydrogen Adsorption in Microporous Metal-Organic Frameworks
• Destabilized $LiB_4$ / $MpH_2$ for Reversible Hydrogen Storage
• Simulation of the Rapid Charging of a Metal Hydride Hydrogen Storage System
• High Capacity Reversible Hydrogen Storage Material

**Animal & Plant Cell Culture Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Metabolic Engineering of *Artemisia Annua* Hairy Roots
• Engineering Microbial Factories for the Production of Plant-Specific Flavonoids
• The Transient Effect of Jasmonic Acid Feeding along with Orca3 Overexpression in *Catharanthus roseus* Hairy Roots
• Effects of Culture Conditions on Production of *n*-3 Fatty Acid from Green Microalga
• Production of Recombinant Human Gelatin in Rice Cell Cultures
• Quantitative Investigation of Microorganism and Fermentation Kinetics of Medicinal Plants in Mold Bran
• Elicitor Treatment of Intact Plants of Papaver Somniferum, and Comparison of Morphinan Alkaloids Production, Gene Transcripts and Protein Expression Profiles upon Elicitation
• Transient Expression of Functional Human Alpha-1-Antitrypsin in *Nicotiana benthamiana* Plants and Suspension Cultures
• Purification and Characterization of a Recombinant Gelatin Expressed in Transgenic Maize
• In Silico Modeling and Simulation of Mouse Hybridoma Cells for the Enhanced Production of Recombinant Proteins

**Applications of Environmental Catalysis II**
***Hilton San Francisco, Union Square 17 & 18***
• Study on the Adsorption Performance of Fe/ZSM-5 and Influence of $O_2$ Concentration in SCR of NOx with Propylene
• Math-Based Approach to Automotive Emission Control System Development: from Global Kinetics to Microkinetics
• Selective Reduction of $NO_x$ with $H_2$, Co and $Ch_4$ in Synthetic and Real Exhaust Gas of a Lean-Burn Engine
• $NO_x$ and Diesel Soot Abatement over Catalytic Traps Based on Mixed Transition Metal Oxides
• Impact of Low Sulfur Gasoline upon $Nh_3$ and $N_2O$ Emission during Cold-Start of Three-Way Catalytic Converters
• Effect of the Catalyst Mileage on the Oxidation Properties of Pd-Based TWC Contained in WCC near Engine
• Modeling of Soot Oxidation in Diesel Particulate Filters Incorporating Cake Layer Microstructure
• Oxidation of Methanol Using Ozone on Titania-Supported Vanadium Catalyst
• Oxidation of Hydrogen Sulfide in Coal Gases to Liquid Element Sulfur Using a Monolithic Catalyst Reactor
• Development of Mixed Phase $Tio_2$ Photocatalysts by Reactive DC Magnetron Sputtering

**Biocatalysis & Protein Engineering Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Directed Evolution of Peptide Conformational Changes
• *De Novo* Protein Design with Flexible Templates and Its Application to the Redesign of Complement 3a
• Investigation of the Applications of Reverse-Phase High Performance Liquid Chromatography in the Structural Studies of Collagen-like Model Peptides
• Fabrication of a Reversible Protein Array Directly from Cell Lysate Using an Elastin-Calmodulin Fusion
• A New Platform Technology for Engineering Intracellular Antibodies Based on the Bacterial Tat Pathway
• Evolutionarily Designed Biterminal Bacterial Surface Display Scaffold
• Identification of T Cell Antigens Using Surface Display
• A Novel Method of Antibody Profiling Using Bacterial Surface Display
• Lipase-Mediated Epoxidation with UHP in Ethyl Acetate
• Discrimination of Peptide Aggregate States in Low Ionic Strength Solutions

**Biological Transport, Migration, and Adhesion Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Fluorescence Resonance Energy Transfer Reveals the Dual Activities of an Integral Membrane
• Kinase/Phosphatase Prokaryotic Porin Regulator in *Escherichia Coli*
• CFD Modeling of Blood Flow in Artery Stenosis
• Regulation of Breast Cancer Migration through Integrin-Cadherin Synergies
• High Laminar Shear-Induced Cyclooxygenase(COx)-2 Promoter Activation Is Mediated by C/Ebpß and C-Jun/Creb in Human Chondrocytic Cells
• Rolling Adhesion Mediated by αL I Domain Mutants
• The Role of Microtubules in Epithelial Cell Rheology
• The Role of F-Actin and Myosin II in Epithelial Cell Rheology
• Role of Phospholipid Signaling in the Gradient Sensing Mechanism of Motile Cells
• Cellular Stress Disrupts Intracellular Transport Machinery
• Protein Extraction by $W_{III}$ System Formed from Binary Aerosol-Ot / Cleavable, 1,3-Dioxolane, Nonionic Surfactants
• Computational Modeling and Experimental Quantitation of Focal Adhesion Formation in Endothelial Cells

**Biomaterials and Tissue Engineering Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Role of Extentional Forces in Targeted Microparticle Adhesion
• A Micro-Fluidic Adipose Reactor for 3-D Localization of Heterogeneous Cell Components
• Chondrocytic IGF-1 Signaling within a Degradable Biomaterial
• Effects of the Production Conditions on the Properties of Fibrous Chitosan-Alginate Membranes Designed for Skin Burn Repair
• Polymer-Tethered Ligand-Receptor Interactions between Surfaces
• Topographic Control of Endothelial Cell Capillary-like-Structure Formation
• Transport Limitations in Islets of Langerhans Culture
• Filtration and Macromolecular Transport in Rat Veins Is Very Different from Its Arteries
• Optimizing Mechanical and Cell Adhesion Properties of Chitosan through Simultaneous Manipulation of Molecular Weight and Crosslinking
• Effect of Different Intermittent Flow Strategies on Mechanotransductive Signaling and Osteoblastic Differentiation of Bone Marrow Stromal Cells
• Transient Dynamics of a Four State Actomyosin Model of Muscle Contraction
• Fabrication of Combinatorial Cellular Microenvironment Using Photoresist Lithography and Protein Microarraying
• Red Blood Cells Enhance the Adhesion of *Staphylococcus Aureus* to Platelets in Shear Flow Via a Chemical and Physical Mechanism
• Improvement of Cell Proliferation on 3d-Scaffold with a Perfusion Bioreactor
• Direct Observation on Bactiseal ™ Catheter by Scanning Electron Microscopy – 4 Cases Studies
• Robustness and Optimality in Developing Organisms
• The Atomic and Electronic Structures of Crystalline Cellulose Iß from First-Principles Calculation
• Dynamic Stem-Cell Culture in Bubble-Confined Cell Array
• Integrated 3d Expansion and Osteogenic Differentiation of Murine Embryonic Stem Cells in a Simulated Microgravity Bioreactor
• Novel Approaches of Scaffold Sterilization and

Cell Seeding for Tissue Engineering Application
• Combination of Proteins on PHßV Microsphere Scaffold to Regulate Hep3ß Cells Activity and Functionality for an in Vitro Model of Liver Tissue Engineering
• Design of Porous Media for Biomedical Applications
• Micropatterned Substrates That Direct Neuronal Polarity

### Biomaterials III
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Incorporation and Release of Hydrophobic and Hydrophilic Bioactive Agents Using Novel Microfiber Scaffolds Produced through Electrostatic Processing
• Nitric Oxide Generating Coatings for Implantable Biomedical Devices
• Engineering of Novel Drug Delivery Devices Based on Convex/Concave Geometries and Dynamic Analysis Using X-Ray Tomography
• Influencing Chondrogenic Differentiation of Hmsc Photoencapsulated in Peg-Peptide Thiol-Methacrylate Mixed Mode Networks
• Hypoxia Increases Proliferation and Adhesion of Human Umbilical Vein Endothelial Cells on Synthetic Graft Membranes
• Anti-Biofilm Properties of Chitosan-Coated Surfaces
• Characterization of Fibrous Chitosan-Alginate Membranes Produced by Coacervation and Designed for Skin Lesion Therapy

### Biomimetics I
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Polysaccharide Hydrogels as Variably Elastic Cell Culture Substrates
• Fibroblast Migration on Covalent Laminin Peptide Gradient Surfaces
• Morphogen Gradient Patterns within Three-Dimensional Matrices to Direct Stem Cell Responses
• Biomimetic Osteoinductive in Situ Crosslinkable Poly(Lactide) for Bone Regeneration
• Supported Bilayers Incorporating Cell-Adhesive RGD Peptides: Composition, Structure and Function
• Design of a Novel Fibronectin-Mimetic Peptide-Amphiphile for Functional Biomaterials

### Biosensors Poster Session
***Hilton San Francisco, Grand Ballroom B***
• Detection of an Ovarian Cancer Biomarker Using Biotinylated Single-Chain Fv with a Surface Plasmon Resonance Sensor
• Behaviorally Induced Glutamate Release Detected in Real-Time with Implanted Biosensor
• Fractal Analysis of Binding and Dissociation of Analytes Related to Human Health on Biosensor Surfaces
• Red Fluorescent Proteins and Their Applications

### Carol in Thermoland II: A Session in Honor of Carol Hall's 60th Birthday
***Hilton San Francisco, Imperial B***
• The Two Aspects of the Protein Folding Problem
• Dynamical Processes in the Small-Numbers Limit
• Structure, Dynamics and Thermodynamics of Water Confined by Surfaces with Patterned Hydrophobicity
• Poly-Q Peptides and Proteins
• Colloidal and Conformational Stabilities of Model Therapeutic Antibodies
• Role of Hydrophobe Distribution on the Thermal Gelation of Biopolymers—Experiments and Simulations

### Catalytic Fuel Processing
***Hilton San Francisco, Continental 2***
• Kinetics and Reaction Mechanism for Ceria Supported Gold Water Gas Shift Catalysts
• Hydrogen from Non-Volatile Biomass Using Autothermal Flash Thermolysis
• Characterization of Nickel-Olivine Materials as Tar Cracking Catalysts in Biomass Gasification Applications
• Cracking of Lipid Molecules by a Superacid
• Production of Light Olefins through Gas Oil Cracking
• Continuous Production of Light Olefins and/or $H_2$ Selectively from Heavy Hydrocarbon Fuels in a Single Compact Reactor
• Ring Opening of 1,3-Dimethylcyclohexane: Effects of Ni and K on Supported Iridium Catalysts
• Direct Coupling of Bromine-Mediated Methane Activation and Coal Gasification: AlB3 Assisted Conversion of Methyl Bromide to Light Hydrocarbons and Quantitative Catalyst Regeneration

### Catalytic Hydrogen Generation for Fuel Cell Applications I
***Hilton San Francisco, Continental 3***
• Monometallic Pd Supported on Zno: Highly Selective Towards CO2 in Steam Reforming of Methanol
• Improved Co Oxidation Activity in the Presence and Absence of Hydrogen over Cluster-Derived $PtFe/SiO_2$ Catalysts
• Evidence of Enhanced Low Temperature Water-Gas Shift Rate with Sodium Promoted Pt/Zirconia-Based Catalysts Discovered by Combinatorial Methods
• Catalytic Conversion of Ethanol to Hydrogen Using Combinatorial Methods
• Activity and Relevant Spectroscopic Features of Gold-Ceria Catalysts for the Catalytic Oxidation of Carbon Monoxide
• Comparative Catalysis Testing and Competing Mechanisms in Methanol Reforming
• Hydrogen Generation from Methanol Oxidation on Supported Pt and Cu Catalysts

### Department Heads Forum
***Hilton San Francisco, Mason***

### Diffusion in Polymers II
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Molecular Dynamics Simulation of Structure, Thermodynamic, Dynamic and Hydrocarbon Permeability Properties of Silicon-Containing Elastomers with Promising Membrane Material Behavior
• Determination of Oxygen Diffusivity(D) and Solubility(k) of a Highly Oxygen-Permeable Soft Contact Lens
• Multicomponent Transport of Water and Methanol in Nafion®
• Computational Study of Water and Toxins Permeability in Sulfonated SIBS Copolymers
• Translational and Rotational Diffusion of Globular Protein in Concentrated Polymer Solutions
• A Novel Universal Diffusion Model for Gas and Solvent Molecules in Polymer
• Increased Mobility in Polypropylene at Intermediate Stereochemical Compositions by Dynamical Monte Carlo

### Downstream Processing Poster Session
***Hilton San Francisco, Grand Ballroom B***
• A Novel Cascade Membrane Bioreactor Configuration for Continuous Production of F(Ab')2 from Igg by Pepsin Digestion
• A Spouted Bed Bioreactor for Solid State Fermentation for Enzyme Production from Plant Biomass
• Scale-up of Breast Cancer Stem Cell Cultures to Suspension Bioreactors
• The Effect of High Dissolved Co2 on Cell Growth and Productivity in Bioreactors
• Microbial Dynamics in an Absorber-Bioscrubber System Operating under Sequentially Alternating Feeding Regimens
• A New Selection Method for Extracellular Enzyme Improvement Via Evolutionary Methods
• Effect of Furfural, Syringaldehyde and Vanillin on Yeast Growth and Xylitol Biosynthesis
• LC-MS Analysis of Degradation Products in Pretreated Biomass
• Flocculation Enhanced Centrifugation and Microfiltration of *Escherichia Coli* Lysate

### Drug and Gene Delivery Poster Session
***Hilton San Francisco, Grand Ballroom B***
• Design of Improved Permeation Enhancers for Transdermal Drug Delivery Part I – Model Development
• Isolation, Amplification and Detection of Viral RNA
• Electrokinetics Assisted Gene and Drug Delivery to Mammalian Cells through a Micro-/Nanoporous Device
• Developing Novel Inhalation Formulations: a Microscopic Approach
• Development and Production of Oil-in-Water Vehicles Microemulsion for Dermal Application of Ectoin
• Bioavailability Estimation of Alginate/Chitosan Capsules Using a Simulated Human Intestinal System
• Mathematical Modeling of the Transdermal Drug Transport Based on Transient Diffusion Trough Homogeneous Membranes
• Analysis of Heat-Aided Membrane-Controlled Drug Release
• Elastic Moduli of Unilamellar Ether-Lipid Vesicles Estimated Using Multi Angle Laser Light Scattering

### Dynamics and Modeling of Particulate Systems II
***Hilton San Francisco, Franciscan D***
• Eulerian CFD Model for Cohesive Frictional Flow
• 3d Simulation of Packed Particle Bed and Transport Properties Prediction for Product Optimization through Virtual Experiments
• Quantitative Characterization of Particulate Materials from Microtomography Imaging
• Modeling Granular Segregation during Hopper Discharge
• Optimization of a Fluid Bed Dryer by the Implementation of a Model Predictive Controller
• DEM Simulations of "Dry Cohesion" Effects in Powder Compaction
• Sedimentation Velocity and Viscosity of Dilute Solid-Liquid Suspensions

### Energetic Materials: Environmental and Life Cycle Issues
***Hilton San Francisco, Continental 9***
• Operational Experience in Photocatalysis: Treatment of Pink Water, Nitroglycerine & Chemical Warfare Agents Using the Photo-Cat® Process
• Biosynthesis of Nitramines
• Environmentally Friendly Green Propellant for the Medium Caliber Training Rounds
• Closed Loop Processing of Energetics to Safely Eliminate Emissions
• Treatment Technologies for Perchlorate
• Waste Treatment Using Molten Salt Oxidation Technology
• Destruction of Tnt and Related Compounds by a Solid-State Monolayer Photocatalyst

### Engineering Treatment and Analysis of Diseases Poster Session
***Hilton San Francisco, Grand Ballroom B***
• Investigating the Mitochondria's Role in the Oxidative Stress of Baculovirus-Infected Cells
• A Chemically Inducible *Cucumber Mosaic Virus* Amplicon Expression System for Production of Recombinant Human Therapeutics in Transgenic Plant Cell Cultures
• Modeling the Mechanism of Drug Transport to Solid Tumors
• Cellular Libraries of Peptide Substrates (Clips): a Method for Rapid Protease Characterization
• Effects of Retinoic Acid on Hepatocyte Morphology, Proliferation and Function
• A New De Novo Approach for Optimizing Peptides That Inhibit HIV-1 Entry
• Using 3-D Tissue Model in High-Throughput Screening: Key to Improve Drug Discovery
• Donor Variation in Proliferation and Multipotency of Human Bone Marrow Stromal Cells
• Evaluation of Leukemia Chemotherapy Using Sto-

chastic Equations of Population Balance Models
• Effects of Flavonoids from Recombinant Microorganisms on Pancreatic ?-Cell Insulin Regulation
• Microscopic and Coarse Grained Stochastic Simulation of Epidermal Growth Factor Receptor Diffusion on Corralled Membrane Surfaces
• Modeling Cellular Immortality in Cancer Cells
• Enhanced Tumor Oxygenation with Hemoglobin Based Oxygen Carriers
• Immunoconjugates and Quantum Dot-Peptide Assemblies for the Detection and Ablation of Advanced Prostate Cancer Cells

**Experimental Methods in Adsorption**
***Hilton San Francisco, Powell***
• Investigation of Adsorption Equilibria of Pure Gases (Co,$CO_2$,$Ch_4$) and Their Binary and Ternary Mixtures at T=293 K for Pressures up to 1.1 Mpa on Activated Carbon (ACAL)
• Sorption Measurements of Alkanes on Zeolites under Equilibrium and Non-Equilibrium
• Ultra-Low Concentration Adsorption Equilibrium for *n*-Alkanes on BPL Carbon
• A Low Cost Sorption Experiment Designed for the Support of $H_2$ Storage Materials Development
• The Partial Loading Zero Length Column Experiment
• X-Ray Microtomography: a Useful Method to Study the Dynamics of Organic and Water Vapors Adsorption on Carbon Filters
• Protein Transport in Charged Agarose Gels Studied by Optical Microscopy in Microfluidics Devices

**WEDNESDAY, 15 NOVEMBER 2006**
***3:15 PM - 4:45 PM***
**FPBE Division Forum**
***Hilton San Francisco, Imperial A***

**WEDNESDAY, 15 NOVEMBER 2006**
***3:15 PM - 5:45 PM***
**Fuel Cell Portable Power Systems II**
***Hilton San Francisco, Continental 8***
• Model Predictive Control for Embedded Applications
• Electroosmotic Pumps for Fuel Delivery to Direct Methanol Fuel Cells
• Composite Membranes for Micro Fuel Cells
• Composite Bed Configuration for Organic Sulfur Removal from Model Logistical Fuel by Using Microfibrous Entrapped Adsorbent
• Synthesis of Hierarchically Structured Zeolite Monoliths as Desulfurization Adsorbents for Logistics Fuel
• Nanoimprinted Electrodes for Micro Fuel Cell Applications

**Fundamentals of Supported Catalysis III**
***Hilton San Francisco, Franciscan A***
• Controlling the Molecular Structure and Reactivity of Supported Metal Oxide Catalytic Active Sites
• ODH of Propane over Several $V_2O^5/TiO_2$-$SiO_2$ and $V_2O_5/TiO_2$ Catalysts: Understanding the Structure-Reactivity Relationship
• Low Temperature Selective Catalytic Reduction of NO by Co over Titania Supported Catalysts
• Effects of Zeolite Structure and Composition on the Synthesis of Dimethyl Carbonate by Oxidative Carbonylation of Methanol on Cu-Exchanged Y, ZSM-5, and Mordenite
• Acid/Base Investigations of Thermally Decomposed Acetylacetonates Supported on Nanocrystalline MgO
• Support Effects on the Catalytic Decomposition of $N_2O$ to $N_2$ over Supported CuO Catalysts

**Gerhold Plenary Session**
***Hilton San Francisco, Yosemite A***
• Membrane Processes—a Disruptive Technology?
• The Challenges in the Synthesis of Multicomponent Configuration in Chemical Industry
• Tunable Solvents for Sustainable Technology
• When Crystalline Solids Are Wanted in Specific Sizes, Forms, and Purities
• Searching for Protein Adhesion-Resistant Membranes with Minimal Misfolding

**Green Biotechnology Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Enzyme Mixtures & Synergistic Additives for Hydrolysis of AFEX Treated Lignocellulosics Using Rapid Microplate Screening Method
• Designer Yeast for Low-Cost Arsenic Removal
• On the Reactivity of Cellulose in Enzymatic Hydrolysis
• Lipoxygenase Catalyzed Production of Monools from Linoleates
• Engineering *Deinococcus Radiodurans* R1 Phosphate Metabolism for Metal Precipitation in Radioactive Waste
• Modeling of a Fungal Biofilter for the Abatement of Hydrophobic VOCs
• Numerical Simulation of Ozone Transport and Uptake in Asymmetrically-Branched Airways of the Respiratory Tract
• Supercritical Carbon Dioxide-Based Cleaning and Sterilization of E. Coli and S. Aureus Biofilms from Stainless Steel Substrates
• High Cell Density Cultivation of Rhodococcus Erythropolis Lsse8-1 for Petroleum Biodesulfurization by Taguchi Doe Methodology
• Process Uniformity of Convective and Diffusive Transport of Heat in Different High Pressure Systems
• Green Biocide Enhancers Enhanced the Biocide Inhibition of the Growth of Sulfate Reducing Bacteria
• Fuel-Grade Ethanol Using New Technologies
• Potential Environmental Application of Self-Assembled Protein Hydrogel Based on Elastin-like Protein Sequences
• Ethanol from Sugar Cane Bagasse by a Simultaneous Saccharification and Fermentation Process (SSF) with Candida Krusei Icm-Y-05
• Towards Continuous Biopesticide Production in Insect Cell Culture: Overcoming Mutations in Fp25k Baculovirus Gene
• Secretion of Recombinant Lignin Peroxidase in the Yeast *Kluyveromyces Lactis*
• Solvent Tolerant Enzyme and Microbial Systems for Biocatalysis
• A Comparative Study of the Effect of Galacto-Oligosaccharides (GOS) on *in-Vitro* Growth of Selected Probiotic Bacteria
• Development of a Mechanistic Model for Sugar-Utilization Regulatory Systems
• Novel Approach for Conversion of Xylose to Ethanol
• Preliminary Evaluation of Anaerobic Production of Aminolevulinic Acid by Methanogens and Acetogens
• Structure and Activity of a Microbial Community Treating Acid Mine Drainage
• Biomimetic Catalysis for Hemicellulose Hydrolysis in Corn Stover

**High Throughput Experimentation**
***Hilton San Francisco, Franciscan C***
• Triple Function Ru Catalysts for Low-Temperature Co Oxidation, VOC Combustion and SCR-Denox
• Discovery and Optimization of NSR Catalysts Via High-Throughput Experimentation
• High-Throughput Metal Nanoparticle Catalysis by Pulsed Laser Ablation
• High Throughput Experimentation (HTE) Applied to Methanol-to-Hydrocarbons Reactions

**Interfacial Phenomena in Conducting and Semiconducting Systems**
***Hilton San Francisco, Union Square 5 & 6***
• Electrochemistry of Active Metals in Aqueous HF
• Interfacial Phenomena in Copper Galvanic Displacement Onto Silicon
• The Electronic Structure of Metals on High-K Dielectrics; Metal Induced Gap States for the Ru and $RuO_2$ on $HfO_2$ Interfaces
• Non-Lithographic Microetching of Transparent Conductive Oxides (Ito and ZnO) and Semiconductors (Gaas) Based on Reaction-Diffusion
• Synthesis of Stabilized Nanoparticles of Varying Composition and Aspect Ratio for Extrinsic Conducting Polymer
• Surface Chemistry of CdSe: Implications for Nanocrystalline Growth

**Mesoscale and Nanoscale Thermodynamics II**
***Hilton San Francisco, Union Square 22***
• Reaction Ensemble Dissipative Particle Dynamics: Mesoscale Simulation of Polymer Reaction Equilibria
• Coarse-Graining Binary Reactive Mixtures to Effective One-Component Systems: from Hard Spheres to Globular Proteins
• Coil and Helical Conformations of Poly(Ethylene Oxide) and Poly(Ethylene Imine) in Solution
• Liquid Crystalline Gel Induced by Ionic Flow
• Modeling of Driven Assembly of Particles in Liquid Crystals: Applications to Optical Sensors and Colloidal Dispersions
• Interfacial Properties and Structure of Complex Fluids from Interfacial-Salt (ISAFT) Density Functional Theory
• Metastable Mesoscopic Clusters in Solutions of Sickle Cell Hemoglobin

**Metabolic Engineering & Systems Biology Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• To Build a Microbial Factory: Investment Cost and Operating Cost Analysis of Metabolic Networks
• Optimization of Stochastically-Simulated Gene Network Models
• How External Electrical Stimuli Can Act at Cellular Level in an in Vitro Culture: Mathematical Model and Experimental Analysis
• A Quantitative Model of Error Accumulation during Pcr Amplification with Application to Gene Synthesis
• Modeling a Subset of Transcriptional Regulatory Network Involving Apoptosis-Related Genes
• Reverse Engineering of an Erythromycin Overproducing Strain
• Gene Expression Profiling of 3t3-L1 Adipocytes Expressing the Mitochondrial Uncoupling Protein 1
• Simulation of Directed Evolution Experiments
• Combinatorial Engineering of Intergenic Regions to Tune Expression of Multiple Genes in Operons
• Complex Systems Analysis and Mathematical Modeling of Insulin Resistance in Skeletal Muscle Cells and the Impact of Plasma Free Fatty Acids
• Identification of Succinic Acid Tolerance Genes in *E.Coli*
• Genome-Wide Transcriptional Response of Staphylococcus Aureus to Hypochlorite-Induced Oxidative Stress
• Optimal Combinatorial Library Design from a Computational Complexity Perspective
• Control of Cell Growth and Glucose Uptake Rates by Controlled Expression of Phosphofructokinase (Pfk) in B. Subtilis
• Selections from Screens: a Novel Tool for the Selection of Overproducers
• Regulating Phenotypic Variations Using Integrated Flux and Energy Balance Analysis Based Multiobjective Framework
• Setting up a High Throughput Screening Facility as Part of the Academic Experience
• Real-Time Detection of TCA Cycle Anaplerosis in Human Glioma Cells with 13c NMR Spectroscopy
• Usefulness of RNAse III Cleavage Sites for Tuning Relative Gene Expression
• Quantifying the Metabolic Capabilities of Engineered *Zymomonas Mobilis* for Ethanol Production from Hexoses and Pentoses Using Linear Programming Analysis
• Translational Coupling and Regulation in Prokary-

otic Operons
• Genomic-Based Identification of the Sporulation Restoring Gene in Degenerate Clostridium Acetobutylicum Strains
• Magnetically Driven Mixing within a Microarray Geometry Using Functionalized Magnetic Nanoparticles
• Nuclear Receptors Based Modulation of Hepatic Lipid and Glucose Metabolism
• Biosynthesis of Lovastatin in a Heterologous Host
• "Retrobiosyntethic" Design for the Microbial Production of an Organic Compound
• Significance Analysis of Time-Series High-Throughput Transcriptional Profiling Data: Applied to *Arabidopsis Thaliana* Liquid Cultures Subjected to Environmental Stresses
• Metabolic Flux Map of E. Coli PTSG Mutant and Wild Type Consuming Glucose/Xylose under Anaerobic Condition
• Development of a Database Tool for Novel Biosynthetic Pathway Design
• Data Correction, Normalization and Validation for Enhanced Accuracy of GC-MS Metabolomic Analysis: Time Series Metabolomic Analysis of *Arabidopsis Thaliana* Response to Elevated $Co_2$ a Case Study
• User-Controlled Changes in Fluorescence Distribution in Cells with Oscillatory Genetic Network Dynamics
• E. Coli Autoinducer 2 Uptake Could Be Induced by Intracellular Factors Such as Luxs Rate but Not Necessarily by the Cell Density: Analysis of the Network Topology Using Bifurcation Analysis
• Sensitivity Analysis on $MS_2$ Viral Dynamics Using Interval Mathematics
• Computational and Recombination Based Methods for Directed Evolution
• A Metabolic Modeling Approach to Optimizing Recombinant Protein Production in *L. Lactis* Fermentations
• Design of Transient Isotopic Labeling Studies for the Experimental Measurement of Autotrophic Metabolic Fluxes
• Shotgun DNA Microarray-Based Transcriptional Analysis of the Clostridium Tyrobutyricum Wildtype and Mutants
• The Bioactivity of Il-12: There's More to the Story Than P70 or P40
• An Age-Structured Model of Dendritic Cell Trafficking in the Lung
• Modeling of Glycolytic Pathway Using in Vitro Kinetics

### Molecular Modeling of Fuel Cells and Electrochemical Systems I
***Hilton San Francisco, Union Square 25***
• Efficient Surface Chemistry Simulations and Applications to PEM Fuel Cell Electrochemistry
• A First-Principles Analysis of Electrocatalytic Oxidation of Co at the Dmfc Anode
• A Density-Functional Theory Study of Hydrogen Underpotential Deposition on Platinum Electrode
• Theoretical Study of the Adsorption/Dissociation of Oxygen on Pt(111) in Electric Double Layer (EDL) for a PEM Fuel Cell
• Dissolution of a Platinum Catalyst in Acid Medium: Density Functional Theory Study
• Near-Surface Alloys for Improved Electrocatalysis
• Modified-Methanol Dehydrogenase Enzymatic Catalysts for Fuel Cell Applications
• Molecular Dynamics Analysis of Methanol Crossover for Direct Methanol Fuel Cells

### Nanotechnology in Water Quality Analysis and Water Treatment
***Hilton San Francisco, Plaza B***
• Mechanism of Arsenic Removal in Electrocoagulation
• Aggregation and Deposition Kinetics of Fullerene Nanoparticles Onto Quartz Surface
• Modeling Interfacial Interactions between Spherical Particles and Nano-Structured Membranes
• SERS-Active Silver Nanoparticle Arrays on Track Etch Membrane Support as Flow-through Water Quality Sensors
• Synthesis and Characterization of Tfc Membranes for Water Reuse
• Synthesis and Characterization of Modified Titanium Dioxide Materials

### New Faculty Forum
***Hilton San Francisco, Van Ness***
• Dr. Judy Raper: National Science Foundation Funding
• Dr. Mike Malone (Dean, UMass Amherst): Engineering Your Tenure

Panel Discussion
• Panelist: Margot Vigeant, Bucknell University
• Panelist: Mario Eden, Auburn University
• Panelist: Mia Markey, University of Texas, Austin
• Panelist: Victor M. Ugaz, Texas A&M University

### Nonlinear Control Design, Analysis and Applications
***Hilton San Francisco, Taylor***
• Nonlinear Controller Design Via Approximate Solution of Hamilton-Jacobi Equations
• A Robust and Stabilizing Multi-Model Predictive Control Approach to Command the Operation of Distributed Process Systems
• Cell and Iterated Dynamic Programming - a Fast Optimizer for Nonlinear Model Predictive Control
• Large-Scale Adaptive Multivariable Controllers Eliminate Step Tests and Maximize Profit
• Design and Performance of an Explicit Parametric Controller for a Solid Oxide Fuel Cell (SOFC) System
• Controlling Weight-on-Bit near Its Optimum in Hydrocarbon Drilling Operations Using a Linear Model Predictive Control with State Estimation
• A Passivity Based Approach to Process Controllability Analysis

### Nonlinear Dynamics and Pattern Formation
***Hilton San Francisco, Continental 1***
• Computation of Equilibrium States and Bifurcations in Chemical Reactor Models Using Interval Analysis
• Capturing Patterns and Symmetries in Time-Periodic Granular Flow
• Application of the Correction Function Method to Solve the Poisson Boltzmann Equation in Unbounded Electrostatic Conditions
• Spatiotemporal Control of Cardiac Alternans
• Nonlinear Behavior of PEM Fuel Cells Operated in Auto-Humidification Mode
• Analysis of Elastic Stability and Structural Response of Cubic Crystals under Uniaxial Loading

### Pharmaceutical Technology Poster Session
***Hilton San Francisco, Grand Ballroom B***
• An Ontology-Based Information Management System for Pharmaceutical Product Development
• Optimization of Solvent Chasing Distillation in Pharmaceutical Industry
• Protein Stabilization by Chemical Stabilizers: Molecular Dynamic Simulation and Experimental Validation
• Development of a Robust Process in Bioreactors
• Trouble-Shooting of Glassy and Ball Material Formulation during Drying of API Wet Cake
• Optimization of Monoclonal Antibody Production Using Process Simulation and Scheduling Tools
• A Systematic Design Approach to Tailor Crystal Size Distribution for Mixing-Sensitive Crystallization Processes
• Inverse-Qsar for Inhibitors of Phosphate Cdc25b
• Elucidating Tablet Movement in a Side-Vented Pan Coater by Digital Video Analysis
• Measuring and Simulation of the Concentration Profile of Binary Mixtures of Powders When Flowing between Flat Plates with Rough Surfaces
• Application of Raman Microscopy and Band-Target Entropy Minimization to Identify Trace Compounds in Model Pharmaceutical Tablets
• The Effect of a New Pressure Change Technology on Microorganisms, an Innovate Concept for Food and Pharmaceutical Safety
• Catalyst Trap Microreactor for Pharmaceutical Hydrogenation Reaction
• Linear Mixed-Effects Models in the Mathematica® Environment
• Operational Challenges of Large Scale Monoclonal Antibody Bulk Production for Clinical Trial Delivery
• Phytochemical Composition and Antimicrobial Activity of the Essential Oil from Echinophora Platyloba DC
• Mechanical Property Characterization of Active Pharmaceutical Ingredients

### Population Balance Modeling for Particle Formation Processes II: Nucleation, Aggregation and Breakage Kernels
***Hilton San Francisco, Union Square 14***
• Analysis of a Moment-Based Inverse Problem Solution Technique for Breakage Kernel Identification
• Population Balance Equation Modeling of Pharmaceutical Emulsions Prepared with High Pressure Homogenization
• Direct Quadrature Method of Moments for Turbulent Aggregation of Fine Particle Populations
• Breakage Distribution Functions Based on Branching Crack Models
• Formulation and Validation of Bivariate Population Balance Models
• A Novel Free Boundary Algorithm for the Solution of Cell Population Balance Models

### Principles of Micropatterned Structures and Applications to Biomems
***Hilton San Francisco, Continental 4***
• Microfabrication of Functional Gels and Application to Controlled Drug Release Microchip
• Influence of Micropatterned Polymer Substrates on Neural Stem Cell Growth and Differentiation
• Optical Microfluid Control Based on Photoresponsive Polymer Gel Microvalves
• Polymer Particle-Based Micromolding to Fabricate Novel Microstructures
• Parallel Manipulation of Adhering Living Cells Based on Photo-Induced Cell Capturing
• Zein Self-Assembly on Nano- and Micro- Patterned Hybrid Surfaces

### Process Design
***Hilton San Francisco, Union Square 24***
• A Simple New Concept for Chemical Process Flowsheet Design and Analysis
• Synthesis of Heat-Integrated Separation Sequences Involving Heat-Pumping
• Quantifying the Effect of Process Design on Controllability and Operability
• A Software Tool for Assessing the Financial and Technical Impacts of Changing Industrial Bio-Manufacturing Processes
• A New Physical Absorption Process for the Capture of $CO_2$ from $CO_2$-Rich Natural Gas Streams
• Cascade Analysis Technique for Targeting Property-Based Material Reuse/Recycle Network
• Attainable Region Construction for Reactor Networks Exhibiting Limit Cycles

### Rational Catalyst Design II
***Hilton San Francisco, Franciscan B***
• Model-Based Design of Single-Site Olefin Polymerization Catalysts
• Multiscale Model-Based Design of Experiments and Catalysts
• Rational Design Supplemented by Serendipitous Discovery – Highly Active and Enantioselective Support-Tethered Co(III)-Salen Complexes for the Hydrolytic Kinetic Resolution of Epoxides
• Grafted Calixarenes for Rational Design of Catalysts and Adsorbents
• Electrostatic "Nano-Engineering" of Promoted and

Bimetallic Catalysts
• Combined Group Contribution and Structure-Activity Relations for Ga/H-[Al]ZSM-5 Catalyzed Dehydrogenation of Alkanes Using Density Functional Theory
• A Novel Computational Framework for the Rational Design of Shape Selective Separation and Catalysis

**Self Assembly in Solution II**
***Hilton San Francisco, Union Square 3 & 4***
• Biocompatible Surfactants for the Hydrofluoroalkane|Water Interface
• Interactions of Dilauroylphosphatidylcholine (DLPC) Lipid Vesicles with Albumin in Aqueous Solutions
• Fluorescence Anisotropy in Aggregated Protein-Mimetic Structures
• Polymer-Surfactant Interactions in Mixed Aqueous Solvents
• Alkaline/Surfactant Process for Enhanced Oil Recovery
• Self-Assembly of Metal Soap Molecular Patterns on Graphite
• Solution Properties of Polysaccharides in Water and Polar Organic Solvents

**Separations Interactive Networking Poster Session Room Setup**
***Hilton San Francisco, Yosemite B+C***

**Structure and Properties of Polymers III: Dynamics of Glass Formers**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Non-Monotonic Glass Transition Profile in Ultrathin Polymer Films and Spatial Cooperation Towards the Glass Transition
• Monte Carlo Simulations of the Glass Transition in Polyethylene
• Modification of Glass Transition Behavior by Confinement in 1-Dimensional Polymer Nanopatterns
• Effect of Confinement on the Relaxation Dynamics in an Antiplasticized Polymer Melt
• Structure, Dynamics and Gas Transport Characteristics of Rubbery Polymer Networks and Nanocomposites
• Dependence of Physical Properties and Morphology of Acrylate/Epoxy LPNS
• Gradient Copolymers with Continuous Distributions of Nanoenvironments Yield Glass Transition Temperatures over 50-80 K in Breadth

**Supply Chain Optimization**
***Hilton San Francisco, Lombard***
• Adopting Methods from Process Safety to Supply Chain Risk Management
• Short Term Planning of Upstream Natural Gas Supply Chain Operations
• Optimal Supply Chain Redesign and Asset Management Using Genetic Algorithm
• Multiobjective Optimization of Hydrogen Infrastructure System Considering Undeterministic Safety Constraints
• Control-Relevant Demand Modeling for Supply Chain Management
• Supply Chain Design and Planning with Responsiveness Testing - a Two-Level Holistic Approach to an Industrial Case

**Sustainable Biorefineries Plenary (Invited Papers)**
***Hilton San Francisco, Continental 6***
• A Research and Market Pathway to Realize the Potential of Ethanol
• Sustainable Energy and Transportation: Engineering the 21st Century
• Dupont's Biorefinery Vision in Support of Sustainable Biofuels & Biobased Chemicals
• A Refiner's Perspective on the Future of Biofuels
• Technology and Economic Risks Associated with the Forest Biorefinery

**Sustainable Power Systems**
***Hilton San Francisco, Continental 5***
• Conceptual Design and Modeling of Entrained Bed Gasifier
• Process Design of Hydrogen Production from Coal and $Co_2$ Separation
• Production of Highly Concentrated Stream of Hydrogen from Syngas in IGCC Processes
• Futuregen: Stepping-Stone to Sustainable Fossil-Fuel Power Generation
• Numerical Simulation of Green Circulating Fluidized Coal Gasifier with *in-Situ* Fixation of $Co_2$
• Retrol Vision: Preliminary Techno-Economical Analysis
• Working Fluids for Geothermal Orc - Processes

**Technology Roadmap: Pharmaceutical Product Development & Manufacturing II**
***Hilton San Francisco, California Room***
• Technology Roadmap: Process Development
• Technology Roadmap: Manufacturing
• Technology Roadmap: Funding Successes & Next Steps

**The Toxicology of Nanomaterials**
***Hilton San Francisco, Union Square 15 & 16***

**Transport Processes in Nanoscale Systems III**
***Hilton San Francisco, Union Square 21***
• Electrochemical Investigation of Transport through Self-Assembled Nanoporous Silica Thin Films
• Diffusion in Polymer Systems with Moving Boundary
• Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA
• Transport Properties of Hydrophilic and Amphiphilic Molecules in the Two Subspaces of Lipidic Cubic Phases
• Isotachophoresis in Nanochannels
• Cross-Stream Migration of Chain Molecules in Nanofluidic Channels
• Axial Diffusion of Simple Gases in Nanotubes: Modeling and Simulation

**Upstream Bioprocessing Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Ethanol and Succinic Acid Production from Afex-Treated Sugarcane Bagasse and Cane Leaf Matter (CLM)
• Investigation of Response Surface Methodology on the Coenzyme $Q_{10}$ Production by Using Photosynthetic Bacteria
• Transcription Modulation of Recombinant DNA Protein Production in a New *Escherichia Coli* Mutant by Using Various Inducer-Feeding Profiles
• Simulation of Biocorrosion in Pipe Flow Using an Electrochemical Glass Cell Bioreactor with a Rotating Cylinder Coupon
• Enhance L-(+) Lactic Acid Production Using Pelletized Rhizopus Oryzae
• Lactic Acid Fermentation with the Supplementation of Fish Wastes
• Lactic Acid Fermentation by *Rhizopus Oryzae* with Activated Carbon Addition
• Particle Dynamics in a Rotating Wall Vessel Bioreactor
• Effect of Operating Conditions on the Performance of Efficient Succinate-Producing *Escherichia Coli* Strains
• Enhanced Propionic Acid Fermentation from Glucose and Lactose by Immobilized Propionibacterium Acidipropionici Mutants Obtained by Metabolic Engineering

**Water Sustainability and Integrated Water Resource Management**
***Hilton San Francisco, Grand Ballroom A***
• An Optimization Model for Planning Wastewater Reuse in the Chicago Area
• Towards Water Sustainability in the Santa Ana Watershed? Pushing the Limits of Reuse & Recycle
• Water Use Prioritization to Maximize Benefit of Treatment and Minimize Environmental Impact
• Principals of Reusing Municipal and Industrial Wastewater Discharges for Irrigated Agriculture
• Life Cycle Assessment as Applied to Water Reclamation and Reuse

**WEDNESDAY, 15 NOVEMBER 2006**
***6:00 PM - 10:00 PM***
**Separations Interactive Networking Poster Session**
***Hilton San Francisco, Yosemite B+C***

**WEDNESDAY, 15 NOVEMBER 2006**
***6:30 PM - 9:00 PM***
**General Papers on Medical Engineering, Drug Delivery and Therapeutic Systems: Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Tethered pH Responsive Biomaterials for Mucoadhesive Oral Controlled Release Drug Delivery Systems
• Exploration of a Protein Molecular Carrier: Self-Assembly and Stability
• Preparation of Efficient Gene Carriers Using Polyamidoamine Dendron-Bearing Cationic Lipids with Different Alkyl Chains
• DNA-Encapsulation Using Self-Assembled Peptide Architectures
• Supercritical Carbon Dioxide and Sterilization of Medical-Grade Polymers
• Characterizing Transport Enhancement by P(Maa-G-Eg) Drug Carriers in the Presence of Mucus
• Study of Targeted Particulate Adhesion to Cellulose Surfaces Mediated by Bifunctional Fusion Proteins
• Sustained Ophthalmic Delivery of Timolol from Molecular Imprinted Contact Lenses
• Enzymatic Polymerization of Natural Phenolic Lipids and Their Potential Application as Anti-Biofouling Materials
• Enhanced Cell-Seeding into 3-D Scaffolds by Use of Magnetite Nanoparticles for Tissue Engineering
• Preparation of Chromatography Matrices Having Thermoresponsive Polymer Brush Structure
• Mechanical Properties of Microporous Foams of Biodegradable Polyesters Formed Via Thermally Induced Phase Separation
• Preparation of Microspherical Hydroxyapatite Scaffolds
• Effect of Particulate Surfactant on Stability of the W/O Dispersion and Microencapsulation of Water
• Preparation of Acellularized Bone Using Ultra High Pressure Technology for Tissue Engineering
• Cell Micropatterning Using Magnetite Nanoparticles and Magnetic Force
• Development of Novel Cell Separation System Using Poly(*n*-Isopropylacrylamide)-Graft-Polypropylene Non-Woven Membrane with Antibody
• Model Analysis of Oxygen Diffusion/Consumption for Cell Culture System to Optimally Design Scaffold and Microbiochip
• Msc Separation on Bioactive Molecule-Immobilized Column
• On-off Control of Drug Permeation through Antigen-Responsive Gels
• Design of Biodegradable Hydrogel by Nanogel Engineering
• Preparation of Hydrogen Bonding Polymer Structures Using Ultra High Pressure Technology as Drug Carrier
• Preparation of Polysuccinimide Microcapsules with pH-Response of Drug Release
• Protein Encapsulation into Thermo-Responsive Biodegradable Nanospheres
• Novel Iontophoresis System for Delivery of Chemically Unstable Drugs
• Internal Model Control of Blood Sugar with Model Uncertainty
• Identification of Correlation and Uncertainty among Parameters Affecting the Dynamics of Blood Glucose Models: Effect of Experimental

Uncertainty
• Design of Dry Powder Inhalation by a Novel Supercritical Freeze Granulation
• Microencapsulation of Living Cells into 150 Micrometer Microcapsules Using Micro-Airflow-Nozzle
• On the Use of a Ferromagnetic Stent for Implant Assisted Magnetic Drug Targeting
• In Vitro and in Vivo Studies of Staphylococcus Epidermidis Adhesion and Colonization on Modified Silicone Surfaces
• pH-Sensitive Drug Delivery System Formulated by Polymerized Bicontinuous Microemulsions for Sustained Enzyme Release

**Poster Session: Catalysis and Reaction Engineering Division Poster Session**
***Hilton San Francisco, Grand Ballroom B***
• Pd-Leaching and Pd-Removal in Pd-Catalyzed Suzuki Couplings
• The Influence of Physical Interactions on Chemical Reactions in Confinement
• A Silicon Microreactor for *in-Situ* Spectroscopic Analysis of Working NSR Catalysts
• A Theoretical Investigation of Co Adsorption on Pt3sn Alloy
• Optimizing Pd Catalyzed Reactions for Pharmaceutical Production
• Modeling and Simulation of a Pyrolysis Reactor for Slurry Feed
• Molybdenum Carbide-Based Catalysts for Gasoline Steam Reforming
• Engineering Advances in Combinatorial Chemistry Relevant to Heterogeneous Catalysis
• Oxidation of Cyclohexane with Molecular Oxygen Using Macrocyclic Homonuclear Cu Complex Catalyst
• Preparation and Testing of $Ab_2O_4$ Spinels (a=Co, Cu, Mn; B=Fe, Cr) for Methane Combustion in Lean Mixtures
• CFD Simulations of Flow and Heat Transfer in Steam Reforming in a Fixed Bed of Cylinders
• Prediction for the Secondary Reaction of FCC Gasoline by Fnn-Ga Method
• Liquid and Gas Phase Laboratory Testing of 1-Butene Rich Fischer-Tropsch Feed over Solid Phosphoric Acid on Kieselguhr
• Propane Ammoxidation to Acrylonitrile over Vanadia-Based Xerogel/Aerogel Catalysts
• Nanostructured Iron-Titanium Oxide Aerogel Photocatalysts for Energy Conversion
• Catalytic down-Hole Upgrading of Heavy Oil
• Trimerization of Isobutene over Cation Exchange Resins: Effect of Physical Properties of the Resins and Reaction Conditions
• Exhaustive Identification of Stoichiometrically Feasible Pathways for Partial Oxidation of Methanol on Copper-Zinc Catalysts
• Aging of Iron Molybdate Oxide Catalysts during Partial Oxidation of Methanol to Formaldehyde
• Optimization of Invertase Production in a Fed Batch Bioreactor by Neuron-Dynamic Programming
• Kinetic Modeling of Hydrogen Production Via Steam Reforming of Methanol
• Ni3AL Intermetallics Catalyst for Hydrogen Production from Methanol
• Thermogravimetric Analysis of Molten Salts' Kinetics
• Fe-Cu Catalysts for Sulfuric Acid Decomposition in SiB Cycle to Thermochemically Produce Hydrogen
• Selective Positional Isomerization of Butene-2 over Mesoporous Silicates
• Community-Extensible Software and Database for Predicting Combustion Kinetics
• Understanding the Aqueous Phase Oxidation of Hydroxylamine by Nitric and Nitrous Acids Using Computational Chemistry
• Catalytic Performance of Aluminum Incorporated MCM-41 for Synthesis of Diphenylmethane Derivatives from Formaldehyde and Phenol, 2,6-Dimethylphenol, or Aniline
• Effects of Ionic Liquid in the Catalyst Preparation of MgO-$CeO_2$ Mixed Oxide for Dimethyl Carbonate Synthesis Via Transesterification
• Photocatalytic Cu Deposition over Self-Assembled Titania Nanoclusters
• First Principles Based Promoter Design for Heterogeneous Catalysis
• Optimal Inlet Temperature Profile Strategies for Decaying Fixed Bed Reactor
• Experimental Investigation of High Temperature Reaction Kinetics of Hydrogen and Air in Turbulent, Supersonic, Combusting Flows
• Modeling of Droplet-Particle Interaction in the Inlet Zone of a FCC Riser
• Hydroconversion of 2-Methylnaphthalene on Pt/Mordenite Catalysts. Effect of the Acid/Metal
• Balance of the Catalyst over the Main Reaction Pathways
• Computational Studies of Liquid Drop Spreading and Dynamics on Porous Solids
• Mass Transport Effects in Biphasic Ionic Liquid/$CO_2$ Systems for Hydrogenation and Hydroformylation
• Deactivation of $MO_2C/ZrO_2$ Catalyst for Steam Reforming of Methanol
• Selective Catalytic Reduction of Nitric Oxide in Diesel Exhaust
• Oxide-Specific Oxidation States of Oxide-Supported Au Nanoparticles
• Promoting the Preferential Oxidation of Co by Altering the Reducibility of Pt
• Production of Hydrogen by Partial Oxidation of Methanol over Promoted Cu/ZnO Mixed Metal Oxide Catalysts
• Propylene Oxidation under Temperature Cycling Operation
• Hydrodynamic , Mass Transfer Parameters and Modeling of Slurry Bubble Column and Ebulating Bed Reactors Operating under Fischer-Tropsch Conditions
• Physical Solvents for Selective $CO_2$ Capture at Elevated Pressures and Temperatures
• Baeyer-Villiger Oxidation with Hydrogen Peroxide over Zeolite Catalysts
• Non-Catalytic Biodiesel Production from Soybean Oil Using Supercritical Methanol
• Microfibrous Supported Catalysts/Sorbents: High Contacting Efficiency Heterogeneous Contacting Systems
• Catalytic Cracking and Aromatization of C4-C5 Hydrocarbons over ZsM-5 Zeolite: Activity and Regeneration
• Steady-State and Transient CFD Simulations of Moving Bed Reactor with Internal Heat Recovery
• Formation of Liquid Element Sulfur and Gaseous Carbonyl Sulfide by Reacting Hydrogen Sulfide in Coal Gases with Sulfur Dioxide
• Conversion of Mixed Sugars into Ethanol by Recombinant *Corynebacterium Glutamicum*
• The Photocatalytic Effects of $TiO_2$ Impregnated with Transition Metals for Removal of Organic Compounds in Liquid Phase
• Modeling of Condensed Phase Combustion-Decomposition Reaction with Gas Generation
• Wittig Reaction of Synthesizing Liquid Crystal Intermediate by Novel Phase-Transfer Catalysis
• Deactivation Mechanisms of Platinum/Titania Catalysts for Sulfuric Acid Decomposition in Sulfur-Iodine Thermochemical Water-Splitting Cycles
• Investigation on the Platinum-Loaded Nay Zeolite Catalysts for Liquid Phase Conversion of Biomass-Derived Carbohydrates to Hydrogen
• Effect of Ceria on Cu-Zn-Alumina Catalyst for Oxidative Steam Reforming of Methanol
• Catalytic Properties of $Ni_3Al$ Powder for Hydrogen Generation by Methane Steam Reforming
• Liquid Fuels from Lignocellulosic Biomass Using an Induction Heating Process
• Release Behavior of Alkali and Alkaline Earth Metals during Biomass Steam Gasification
• Characterization and Activity of K-, CeO2-, and Mn-Promoted Ni/$AL_2O_3$ Catalysts for $CO_2$ Reforming of Methane
• Thermodynamic Analysis and Reaction Evaluation for the Absorption-Enhanced-Water-Gas-Shift Reaction (AEWGS) for the Production of Hydrogen
• Steam Reforming of Methanol Using Supported Mo2c Catalysts
• Preparation of Mesoporous Clay Complex by $TiCl_4$ Treated with $Nh_4Oh$ for Selective Catalytic Reduction
• A Shape Selective Catalyst for Epoxidation of Cyclic Olefins: the Nanoporous Nickel Phosphate VSB-5
• Investigation of Effective Factors on $V_2O_5$ Catalyst Deactivation in $H_2SO_4$ Production
• Lipase Catalyzed Hydrolysis of Olive Oil in a Biphasic Enzyme Membrane Reactor: Modeling of Mass Transfer Effect
• Monodispersed Pd-Nanoparticles for Selective Hydrogenation

**THURSDAY, 16 NOVEMBER 2006**
***8:30 AM - 11:00 AM***
**(22b) Micro- and Nanodevices for Targeted Therapeutics I**
***Hilton San Francisco, Union Square 24***
• Polymer Core/Gold Nanoshell Composite Nanoparticles for Targeted Therapeutics: Monitoring Their Response to Different Media and Laser Irradiation
• Metal-Polymer Nanocomposites for Therapeutic and Imaging Applications
• Functional Block Copolymer Nanoparticles for Targeted Drug Delivery and Imaging
• Development of Improved Retinal Prosthesis, Using Local Release Polymer Coatings and Sustained Release Dendrimer-Drug Nanodevices
• Functionalized Liposomes for Targeting Colorectal Cancer
• Emerging Nanotechnologies for Therapeutic Applications

**(22b) Nanotechnology for *in Vivo* and *in Vitro* Imaging**
***Hilton San Francisco, Union Square 5 & 6***
• Single-Walled Carbon Nanotube Optical Biosensors of DNA Structure
• Using Peptides to Propel Nanoparticles to the Top of the Nanobio Arsenal
• Nanogold Particle for Enhanced Fluorescent Contrast in Fluorophore Mediated Breast Cancer Imaging
• Molecular Dynamics Imaging in Micropatterned Living Cells
• Two-Photon Excitation Photoluminescence of Spiropyran-Containing Polymer Nanoparticles and Their Imaging Application
• Two-Photon Excitation of Quantum Dot Donors in Fluorescence Resonance Energy Transfer Applications

**Advanced Computations and Numerical Models in Water Technology and Resource Management - II**
***Hilton San Francisco, Plaza B***
• The Role of Simulation in Evaluating Water Purification, Wastewater Treatment, and Recycling Processes in the Semiconductor Industries
• A Retrofit Model of Water Networks in Industrial Processes
• Molecular Simulation of Arsenic Adsorption in Layered Double Hydroxides
• Optimization of Water Networks in Industrial Processes from a Management Point of View
• Bond Graph Modeling of an Integrated Biological Wastewater Treatment System

**Advanced High Temperature Systems and Materials for Hydrogen Production**
***Hilton San Francisco, Union Square 13***
• A Helium Loop for the Transfer of Heat between a Nuclear Reactor and a Thermochemical Plant
• Heat Transfer within a Ceramic Heat Exchanger Used for Sulfuric Acid Decomposition
• Corrosion Performance of Ceramic Materials in

High Temperature Sulfuric Acid Environments
• Materials for Sulfuric Acid Decomposition in the S-I Cycle
• Evaluation of Material Corrosion in Molten Fluoride Salt
• Development of C-Sic Ceramic Compact Plate Heat Exchangers for High Temperature Heat Transfer Applications

### Advances in Biocatalysis and Protein Engineering
***Hilton San Francisco, Franciscan C***
• Using Light Illumination to Control the Form-Function Relationship of Enzymes
• Protein Dynamics and NMR Relaxation: toward a Mechanistic Understanding of Salt-Activation in Nonaqueous Biocatalysis
• Measurement of Endo and Exo-Glucanase Activities in Cellulase Using Non-Crystalline Cellulose
• Immobilization of Bacterial Beta-Galactosidases Onto Nanofiltration Membrane and Its Application on Production and Separation of Galacto-Oligosaccharides
• Understanding the *Lpp* Deletion Effects in Membrane Permeability and Consequences for Whole-Cell Biocatalysis
• Kinetics of the Multienzyme System-Alcohol, Aldehyde and Lactate Dehydrogenase-for the Metabolism of Ethanol to Acetate
• Lipase-Catalyzed Selective Transesterification of Stanols in Solvent Free Medium

### Advances in Drug Delivery I
***Hilton San Francisco, Sutter***
• Therapeutic Proteins and Degradable Polymersomes
• Nanoparticles Targeting Intercellular Cell Adhesion Molecules
• Integrin Antagonist C16y Peptide Encapsulating Pla & Pla-PEO Nanoparticle Treatment of Choroidal Neovascularization in Rodents
• Subconjunctivally Implantable Hydrogels for Prolong Release of Therapeutic Proteins
• Bioerodible Scaffolds for Implantable Microfluidic Probes in Convection Enhanced Neural Drug Delivery
• Low Frequency Sonophoresis: Ultrastructural Basis for Stratum Corneum Permeability Assessed Using Quantum-Dots
• Effect of Microneedle Design on Pain in Human Subjects

### Advances in Electrokinetics and Electrophoresis - DNA Applications
***Hilton San Francisco, Union Square 19 & 20***
• Simultaneous 2d Electrofocusing
• DNA Collisions with a Single Post
• DNA Electrophoresis in Microfluidic Post Arrays under a Moderate Electric Field
• Confocal Laser Scanning Microscopy of DNA Electrophoresis in Microchannels
• Determination of the Effective Charge of DNA Fragments Containing Variable Numbers of A-Tracts
• Enhancement of DNA Hybridization Kinetics by DC Electrokinetic Mixing in Microchannels

### Advances in Metabolic Engineering and Bioinformatics (II)
***Hilton San Francisco, Yosemite B***
• Understanding Cofactor Partitioning in Xylitol-Producing *Escherichia Coli* Expressing Xylose Reductase
• Metabolic Control Analysis Provides Insights into Strategies for Improving Ethanol Production from Recombinant Xylose-Utilizing *Saccharomyces Cerevisiae*
• Simultaneous Estimation of Reaction Fluxes and Metabolite Levels Using Instationary $^{13}C$ Metabolic Flux Analysis
• Total Microbial Synthesis of Benzylisoquinoline Alkaloids in Saccharomyces Cerevisiae
• Forward Engineering of a *S. Coelicolor* Actinorhodin Overproducer Using Transposon Mutagenesis
• Engineering of Organic Acid Tolerance Genes in *E. Coli* for Biorefinery Applications
• Biosynthesis of Fosfomycin

### Advances in Protein Structure, Function, Analysis and Stability - I
***Hilton San Francisco, Powell***
• A Novel Cytokine Recognition Mode in the Structure of Interleukin-2 Complexed with Its Alpha Receptor
• Atomic Resolution Structures of Fkbp12 Wild Type and Mutants Show the Existence of a Coupled Network of Amino Acids and a Structural Water in the Protein Core
• Binding Site Allostery in the *E. Coli* Groel Chaperonin Subunit
• Local Motions in Allosteric Proteins
• A Novel Approach for Alpha-Helical Topology Prediction in Globular Proteins
• An Antibody Loop Replacement Design Feasibility Study and a Loop-Swapped Dimer Structure
• A Branch-and-Reduce Algorithm for the Contact Overlap Problem

### Biomaterials IV
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Field-Driven Surface Biofunctionalization of Electrospun Fibers
• Kinetic Studies of Ntpdase Immobilized on Polyethylene Terephthalate
• Fundamental Studies on the Modification of Silicon Surfaces Using Aptes (3- Aminopropyltriethoxysilane) for Neural Implant Applications
• Surface Science Studies on the Effects of Different Silanes and Metal Surface Treatments on the Binding of Chitosan, a Biopolymer
• Vapor Phase Photografting of Antimicrobial Polymer Coatings
• Surface-Confined Photografting on Pla and Pha Films
• Mechanisms for Controlling Protein Orientation

### Biomimetics II: Drug Delivery
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Intracellular Trafficking and Drug Release Mechanisms of Dendrimer-Based Drug Delivery Nanodevices
• A Model for Polymer Functionalization of Drug Delivery Vehicles: Maximizing Adhesion While Confronting Endothelial Glycocalyx
• Conjugation of Methoxypolyethylene Glycol to the Surface of Bovine Red Blood Cells for Use as a Non-Immunogenic Blood Substitute
• Incorporation of Statins in a Perivascular Polymeric Drug Delivery Device for the Inhibition of Intimal Hyperplasia
• Micro- Electrochemical and Electrophoretic Delivery of Charged Species from Conducting Polymer Surfaces
• Antigenic Disguise of Model Surfaces Via Immobilization of Treponema Pallidum Protein Tp0483

### Bridging Academia and Biotechnology Industry
***Hilton San Francisco, Union Square 21***
• Training Scientists and Engineers for the Biotech Industry: Lessons Learned from an Unexpected Quarter
• Pharmaceutical Engineering Programs and Courses for the Working Pharmaceutical Professionals
• Leveraging Biotechnology Training to a Career in the Pharmaceutical Industry - a Student to an Employee Perspective
• Panel Discussion
• Panel Speaker—Sharfstein
• Pannel Speaker

### Cape-Open Current Status: Extensions and Improvements
***Hilton San Francisco, Union Square 3 & 4***
• Experiences with Cape Open Thermo Interface in Basf in-House Simulator Chemasim
• Aspen Technology's Current and Future Support for Cape-Open Standards
• Interoperability between Modeling Tools (Mot) and Process Simulators (Prosim) through Cape-Open Standards
• Tools Supporting Implementation of Cape-Open Interfaces
• Interoperability of Com/.Net Cape-Open Process Modeling Components and Environments
• Remote Access Networked Models in a Collaborative Power Industry Application

### Cardiovascular and Cancer (II)
***Hilton San Francisco, Yosemite A***
• Scaffold Pore Structure and Mechanical Properties and Their Effects on Tevg Outcome
• Inter-Domain Non-Covalent Interactions Stabilize the Solution Structure of Human Von Willebrand Factor
• Characterization of Peptides Isolated from Bacterial Display Libraries Binding to Tumor Cell Surface Receptors
• Targeting L-Methioninase to the Vasculature of Tumors
• Dendrimer-Based Nanodevices for Targeted Cancer Therapy Based on Mechanistic Understanding of Device Performance
• The Role of Mesenchymal Bone Marrow-Derived Cells in Tumor Formation
• Influence of Toxicity Effects on Model-Based Docetaxel Treatment Design

### Catalytic Hydrogen Generation for Fuel Cell Applications II
***Hilton San Francisco, Continental 3***
• Development of a Monolith Supported Catalyst System for a Miniature Fuel Cell Power Source
• Development of Highly Active Nanoscale Catalysts for Production of CO Free Hydrogen by Dehydrogenation of Methane
• Methane Partial Oxidation over a Rh-Containing Monolith Studied by Spatially Resolved Intra-Channel Species and Temperature Measurements
• Auto Thermal Reforming of LPG over Bimetallic Pt-Ni Catalyst
• Novel Perovskite Catalysts for the Auto-Reforming of Sulfur Containing Fuels
• Hot Reformate Gas Desulfurization Using Regenerable Cerium and Lanthanum Oxide Sorbents
• Sulfur Tolerance of Precious Metals Supported on Ceria-Zirconia Catalyst Supports

### Cell Adhesion and Migration (II)
***Hilton San Francisco, Yosemite C***
• Migratory and Proliferative Effects of Kgf Are Mediated by ERK 1/2 Mapkinase Pathway and Ccaat/Enhancer Binding Proteins
• New Method for Describing Connective Tissue Cell Migration with Persistent Random Walks
• Cell-Cell Mechanical Communication through a Deformable Substrate
• O-Glycosylated Cd44 Variant Isoforms Are the Major Functional P-Selectin Ligands on Colon Carcinoma Cells
• Effect of Blending Chitosan and Gelatin on Cell Adhesion
• Engineering Cell Adhesion Dynamics for Esophageal Tissue Engineering
• Inhibiting *E. Coli* Biofilm Formation with Self Assembled Monolayers Presenting Functional Groups

### Circulating Fluidized Beds
***Hilton San Francisco, Union Square 14***
• Simulation of the Selective Oxidation of *n*-Butane to Maleic Anhydride in a Riser/Regenerator-System
• 3d Steady State Riser Simulations Using Filtered Gas-Solid Momentum Transfer Models
• Correlation of Solids Holdups in the Fully Developed Region of Gas-Solid Two-Phase Flow
• Identification of Standpipe of Cold Flow Circulat-

ing Fluidized Bed System with Minimal Number of Pressure Variables
• Cluster Dynamics in a Circulating Fluidized Bed
• Can Chemical Looping Combustion Use Cfb Technology?

**Complex and Networked Systems I**
***Hilton San Francisco, Van Ness***
• Model-Based Design of Networked Control Systems: Handling Control and Communication Constraints
• Oscillator Synchronization: Cluster Dynamics of a Complex Phase Transition
• Coarse Collective Dynamics of Animal Groups
• The Core and the Most Useful Molecules of Organic Chemistry
• Fault-Tolerant Process Control: Handling Asynchronous Sensor Behavior
• Topological Paradigms for Supply Network Optimization

**Desalination Processes - I**
***Hilton San Francisco, Plaza A***
• Numerical Modeling Mineral Salt Surface Scaling in Reverse Osmosis Modules Using Single Crystal Growth Kinetics
• The Ammonia-Carbon Dioxide Forward Osmosis Desalination Process: a High Recovery Alternative to Reverse Osmosis
• Multiscale Studies of Membrane Distillation of Saline Water-–Experimental Results and Modeling
• Real-Time Mineral Scale Detection and Characterization Using a High Pressure RO *Ex-Situ* Scale Observation Detector
• Evaluating the Scaling Potential in Cross-Flow Membrane Distillation Modules
• High-Efficiency Seawater Desalination Via Nf/RO Multi-Pass Arrays

**Design, Fabrication and Application of Microsensors**
***Hilton San Francisco, Union Square 1 & 2***
• Microfabricated Electrochemical Organophosphate Sensor Based on Oxime Chemistry
• Use of a Silicon Photo-Detector to Probe the Evanescent Field Surrounding a Planar Waveguide Sensor
• Photopatterned Surface Modification of Su-8 Photoresist for Lab-on-a-Chip Applications
• Development of a Platform for the Monitoring of Extracellular Ionic Activities
• Understanding the Reversibility of Carbon Nanotube Gas Sensors
• Hexagonal Saw Device for Evaluation of Polymer Properties
• Direct Printing of Three-Dimensional and Curvilinear Micro-Architectures into Solid Substrates with Submicron Resolution

**Environmental Fate and Transport Processes I**
***Hilton San Francisco, Union Square 15 & 16***
• On the Fate of Xenobiotic Compounds during Alternative Methods of Municipal Sludge Treatment
• Enhanced Biofilm Attachment Onto Polyurethane Foam, Packed-Bed Biotrickling Filters for the Treatment of Odors
• A Method for Modeling Chemical Multimedia Partitioning with Neural Networks and Classifiers
• Nanoscale Iron Remediation of Trichloroethylene Monitored by Microcapillary Microscopy
• Evidence of Natural Attenuation of Hexavalant Chromium in Groundwater Plumes at Tinker Air Force Base

**Fuel Cell Portable Power Systems III**
***Hilton San Francisco, Continental 8***
• Reformed Methanol Micro Fuel Cell Systems for Portable Power Applications
• Novel Chemical Mixtures to Generate Hydrogen for Portable Fuel Cells
• Hydrogen Generation by Reforming Dimethylether Using Micro-Channel Reactor
• Integration Potential in Different Reformer Strategies for Logistical Fuels Processing
• Design and Strategies for Operating PEM Fuel Cells with Dry Feeds

**Fuel Cell Technology III**
***Hilton San Francisco, Continental 7***
• The Oxygen Non-Stoichiometry and Structure of Solid Oxide Fuel Cell Cathode Materials Measured by *in-Situ* Neutron Diffraction
• Sintering Behavior of *in-Situ* Doped Nanoparticles by Flame Spray Pyrolysis for Fuel Cell Applications
• Direct Oxidation and *in-Situ* Reforming of Methane on Ceria Anodes for Solid Oxide Fuel Cells
• Perovskite-Based Catalysts for Dirct Alcohol Fuel Cells
• Oxygen Reduction Kinetics and Surface Chemistry of Doped Lanthanum Ferrites

**Green Chemistry and Engineering for Sustainability**
***Hilton San Francisco, Continental 5***
• I-Messe, a New Evaluation Method for Green and Sustainable Chemistry
• Development of Novel Polycarbonate Melt-Process (Mitsubishi Melt-Process) and Its Assessment from the View Point of Green Sustainable Chemistry by Means of I-Messe
• Evaluating the Sustainability of Green Chemistries: Development of the Greenscope Tool
• The Design for the Environment Green Formulation Initiative
• An Environmentally-Friendly Process for Fuel Cell Electrode Reclamation
• Measurement and Reduction of Organic Solvents in Pharmaceutical Manufacture
• Reaction of Bio-Related Compounds in Hydrothermal Electrolysis
• Mechanism and Pathway of the Water-Soluble Protein Hydrolysis under the Saturated Sub-Critical Water Condition

**Green Chemistry and Reaction Engineering**
***Hilton San Francisco, Franciscan B***
• Expanding the Utility of One-Pot Multi-Step Reaction Networks Via Catalyst Compartmentation and Recovery
• Continuous Reactor Design for Oxidation of Pharmaceutical Intermediates
• Decomposition of Hydrogen Sulfide in a Nonthermal-Plasma Pulsed Corona Discharge Reactor
• Understanding $NO_x$ Storage on $Pt/BaO/Al_2O_3$ Catalysts Using Simulated Diesel Exhaust
• N Vinyl Formamide: Green Alternative to Acrylamide
• Solid-Liquid Phase Transfer Catalyzed Synthesis of Cinnamyl Acetate-Kinetics and Analysis of Factors Affecting the Reaction in a Batch Reactor
• Modeling of Carbonation Reaction Involving Dolomite-Based Sorbents
• Calcium Reclamation and Synthesis of Precipitated Calcium Carbonate for Acid Gas Control in Flue Gas

**Green Processing and Applications Using Ionic Liquids**
***Hilton San Francisco, Union Square 17 & 18***
• Arene Carbonylation in Chlorometallate, Dialkylimidazolium Ionic Liquids: Effect of Changing Metal Chloride
• Enzyme Structure, Function, and Utility in Room Temperature Ionic Liquids
• Designing Green Processes: Phase Behavior of Ionic Liquid - Carbon Dioxide Based Systems
• Using Carbon Dioxide as an Antisolvent Separation Aid with Ionic Liquids: Thermodynamics and Solvent Strength
• Decomposition of Ionic Liquids in Chemical Processing
• Hydrogen Bonds in Imidazolium-Based Ionic Liquids with –Nh2: Ab Initio and Molecular Dynamics Study
• Measurement of the Selective Solubilities of $Ch_4/C_2H_6/CO_2$-Mixtures on Alkylsulphate Ionic Liquids for Natural- and Biogas Cleaning
• Grafted Poly(Ionic Liquid) Membranes for CO2 Separation
• Solubilities and Mass Transfer Coefficients of Gaseous Mixtures in Physical Solvents for $CO_2$ Capture Applications

**Management and Business Issues in Product Design**
***Hilton San Francisco, Union Square 22***
• "Big Gain Hunting: Market Demand as the Pre-Eminent Spec. for Successful Product Design"
• Cost- Effective Creativity – a Partnership between Technology and Commercial Management
• Breaking Barriers to Product Design Team Success (or Stopping Management from Undermining Teams)
• Addressing Patent Protection in the Product Development Process
• Use of Quality by Design Principles in Pharmaceutical Product Development
• Capability Lifecycle Management: Connecting Product Opportunities to Processing Capabilities

**Membranes for Hydrogen Purification**
***Hilton San Francisco, Continental 2***
• Encapsulated Pd Composite Hollow Fiber Membranes: Permeation and Reaction Studies
• Synthesis and Characterization of Thin and Dense Pd-Ag Membranes Supported on Porous Metal Surface
• Sulfur Resistant Metal Alloy Membranes for Hydrogen Purification
• Chemical Stability and Hydrogen Permeation Properties of Zirconium- Doped Mixed Proton-Electron Conducting Strontium Cerate Membranes
• Inorganic Membranes for the Separation of Hydrogen from Coal-Derived Synthesis Gas
• Electrical Conductivity and Chemical Stability of Novel Titanium-Doped Mixed Proton- and Electron-Conducting Perovskite Membranes for Pure Hydrogen Production
• A Novel Characterization of Pd/Ag Alloy Phase Nucleation and Growth Kinetics Via *in-Situ* Time-Resolved High Temperature X-Ray Diffraction Analysis

**Metabolomic Approaches to Systems Biology**
***Hilton San Francisco, Imperial B***
• Increasing the *in Vivo* NADPH Availability by Metabolic Engineering in *Escherichia Coli*
• Elucidating the Mode of Cytotoxicity in an *Escherichia Coli* Strain Engineered for Isoprenoid Production Using Transcriptomics and Metabolite Profiling
• Metabolic Profile-Based Analysis of Metabolic Network Modularity
• Systematic Identification of Conserved Metabolites in GC-MS Data for Metabolomics and Biomarker Discovery
• Accurate Time-Series Metabolomic Analysis of a Systematically Perturbed *Arabidopsis Thaliana* Liquid Culture System for Studying Regulation of Plant Primary Metabolism
• Flux and Transcriptome Alterations in Mammalian Glycerol Kinase Disorders
• Effect of *Yfi*D and *Pox*B Gene Disruption on Microaerobic Pyruvate Catabolization and Metabolic Flux Distributions Based on C-13 Labeling Experiments

**Mixing Issues in Industrial Processes I**
***Hilton San Francisco, California Room***
• Impeller Design for Simultaneous Improvement of Economics and Efficiency
• The Effect of Reduced Baffling on the Mixing Characteristics of a Retreat Blade Impeller Agitated Tank
• Experimental and Computational Determination of the Hydrodynamics in a Stirred Tank Reactor Provided with a Retreat Blade Impeller
• Drawdown of Floating Solids in Stirred Tanks:

Baffle Design to Minimize Power Consumption
• Simulation of Continuous Boric Acid Slurry Reactors in Series by Microfluid and Macrofluid Models
• Interstage Backmixing and Purging Performance of a Multistage Solids Purge Column

### Morphology and Structure
***Hilton San Francisco, Continental 1***
• Semiconductor/Insulator Interfaces in Organic Thin Film Electronics
• The Microstructure Foundation of High Carrier Mobility in Semiconducting Polymers
• Self-Assembly of a Model Semiconducting Rod-Coil Block Copolymer in Thin Films
• Solvent Vapor Annealing Improves Device Characteristics of Solution-Processable Triethylsilylethynyl Antradithiophene
• Alignment and Higher Order Liquid Crystalline Structure in Monodisperse Conjugated Polymers

### Multiphase Reaction Engineering
***Hilton San Francisco, Franciscan A***
• Bubble Dynamics Study in a Slurry Bubble Column with a Four-Point Optical Probe
• Gas-Liquid Reactor Model for the Liquid-Phase Oxidation of Hydrocarbons
• Multiple Hydrodynamic States in Trickle Flow Reactors: Towards Optimizing Reactor Performance by Manipulation of the Hydrodynamic State
• Polymer Hydrogenation by Reactive Extrusion - Pulsed and Continuous Flow Systems
• Multi-Scale Modeling of Selective Oxidation in a Circulating Fluidized Bed Downer Reactor
• Modeling of Trickle Bed Hydro-Processing Reactor
• Acoustic Detection of Flooding in Absorption Columns and Trickle Beds
• Removal of Hydrogen Sulfide in Coal Gases Producing Liquid Element Sulfur

### Multiscale Modeling and Design
***Hilton San Francisco, Union Square 25***
• Target-Oriented Multiscale Systems Engineering with Application in Automotive Paint Spray
• Ultraviolet Absorber Function in Polymers: Multiscale Simulation Starting at the Molecular Level
• Multiscale Modeling and Sequential Design of Experiments
• Implications of Incommensurate Interactions between Perfluorocarbons and *n*-Alkanes
• Time-Scales in Distillation Models
• Multiscale Optimization in Molecular Modeling

### Nanomaterials Process Development and Commercialization
***Hilton San Francisco, Grand Ballroom A***
• Invited Talk: Nanostructured Surface Treatments Enable the Formulation of Nano-Particulates and Acrylate-Based Polymers in Cosmetic Applications
• Invited Talk: the Impact of Nano-Materials on Coatings Technologies
• A Hydrodynamic Method for the Continuous Production of Nanoparticles
• Diamond Molecules: Building Blocks for Nanotechnology
• Industrial Scale Processes for Nanomaterials to Enable Commercial Applications
• Individual Nanoparticle Coating Using Atomic Layer Deposition

### Nanoscale Structure in Polymers I: Self-organization of Polymers at Surfaces and Interfaces
***Hilton San Francisco, Continental 4***
• Double Network Hydrogels, Structure and Response to Applied Stress
• Thermal Spraying of Nylon-11 and Nylon-11/Silica Coatings: Modeling and Characterization of Coating Microstructure
• Light Intensity and Crosslinking Effects on the Nanostructure of Polymerizable Lyotropic Liquid Crystalline Systems
• Sulfonate Functional Nano-Porous Membranes Templated from Ordered Block Copolymers
• Nanometer-Scale Polymeric Structures on Surfaces: Pillars and Honeycombs
• Directed Polymer - Nanoparticle Self Assembly to Manufacture Layered, Nanostructured Materials
• Influence of Strongly Interacting Hompolymers on the Long-Range Order in Semi-Crystalline, Amphiphilic Block Copolymer Templates

### Nanostructured Thin Films
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Patterning of Mesoporous Silica Thing Films Using Traditional Photolithography Techniques
• Metal and Semiconductor Nanowire Network Thin Films with Hierarchical Pore Structures and Its Photovoltaic Applications
• Mechanical Properties of Nanoporous Platinum Thin Films
• Acid-Functionalized Mesostructured Aluminosilica Films for Proton-Exchange Membrane Applications
• Synthesis and Crystallization of Titania Films with Orthogonally Aligned Hexagonal Close Packed Cylindrical Nanopores
• Durability of Hydrophilic and Antimicrobial Zeolite Coatings

### Novel Catalytic Materials
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Towards Tailoring of Highly Active and Stable Nanocomposite Catalysts
• Infusion of Pre-Synthesized Iridium Nanocrystals into Mesoporous Silica for High Catalyst Activity
• Mesoporous and Nanostructured Multicomponent Mo-V-Te-Nb-O Catalysts for Propane Ammoxidation to Acrylonitrile
• Synthesis of Co Incorporated MCM-41 Large Particle Pseudomorphs
• Microwave Synthesis of NTHU-4 and Related Materials
• Structure and Catalysis of V-ZSM5 Prepared by Vapor Exchange of Vanadium (V) Trichloride Oxide
• Silica Nanofiber Mats Containing Transition Metal Oxide Crystals Via Electrospinning and Sol-Gel Synthesis

### Plenary Session on Computational Molecular Science and Engineering
***Hilton San Francisco, Imperial A***
• Equation-Free Modeling for Complex/Multiscale Systems
• Using First Principles Methods to Accelerate Materials Discovery for Hydrogen Production and Storage
• Creating and Harnessing Complex Reaction Networks
• Simulation of Self-Assembly in Colloidal and Polymeric Systems
• Cosmo-RS: from Quantum Chemistry to Fluid Phase Thermodynamics

### Plenary: Frontiers in Alternative Fossil Fuels
***Hilton San Francisco, Continental 6***

### Pretreatment of Lignocellulosic Biomass and Interactions with Other Processing Steps I
***Hilton San Francisco, Continental 9***
• Comparative Data for Enzymatic Digestion of Corn Stover and Poplar Wood after Pretreatment by Leading Technologies
• Pretreatment Conditions and Enzymatic Hydrolysis of Poplar
• Substrate Dependency on the Effect of Pretreatment by Aqueous Ammonia
• Lime Pretreatment of Poplar Wood
• Integration of Biomass Conversion Processing Steps with Advanced Enzymes
• Effect of Fermentation Inhibitors on the Cofermentation of Glucose and Xylose from Pretreated Lignocellulosic Biomass by Recombinant Yeast
• Logistical Support and Modeling Efforts in Pretreatment Research

### Processing and Safety of Energetic Materials
***Hilton San Francisco, Franciscan D***
• Truly Flexible Manufacturing Technologies for the Processing of Energetic Formulations
• Continuous Shear Roll Milling of Gun Propellants
• Twin Screw Extrusion of Aluminized Thermobaric Explosives
• Squeeze Flow Rheometry for Rheological Characterization of Energetic Formulations
• Processing of Nanoenergetics with a Fully-Functional Mini-Twin Screw Extruder
• Real Time Ir Used in Tagzt Synthesis
• Adjustable Gap Rheometry for the Rheological Characterization of Energetic Formulations

### Simulation and Control of Multiscale Systems I
***Hilton San Francisco, Taylor***
• Stochastic Simulation of Catalytic Surface Reactions in the Fast Diffusion Limit
• Temporal Coarse-Graining of Lattice Kinetic Monte Carlo Simulations
• Mass Transport Dynamics, Cell Population Heterogeneity and Domain Geometry Modulate the Architecture of Regenerating Tissues
• Multi-Scale Modeling of Quantum Dot Synthesis in Microemulsions and Liquid Crystals
• Modular Coupling Strategies for Melt Crystal Growth Models
• Multiscale Modeling of High-Shear Granulation Processes

### Site Assessment and Remediation - I
***Hilton San Francisco, Lombard***
• Chemical Characteristics of an Anthropogenic Marine Sediment and Its Biogas Production Potential
• Economic Assessment for Replacement of Granular Activated Carbon Treatment of Groundwater at Two Treatment Plants at Former Kelly Air Force Base
• Chemical Stabilization and Cost Effective Management/Remediation of Target Ranges
• Electrolytic Permeable Reactive Barrier to Control the Flux of Explosive Compounds in Groundwater at the Pueblo Chemical Depot
• Application of Emulsified Carbon Substrate to Soil Excavations to Enhance Biodegradation of Chlorinated Ethenes
• A Five-Year Field Study to Evaluate Phytoremediation of a Crude Oil-Contaminated Soil

### Structure and Properties of Polymers IV
***Marriott San Francisco, Yerba Buena Ballroom 1***
• A Coarse-Grained Gaussian Slip-Link Model for Single and Double Polymer Networks
• Dynamic Prediction of Microstructure and Molecular Size in Coordination Terpolymerizations Including Cross-Linking and Branching
• Stress Generation by Solvent Absorption and Wrinkling of a Cross-Linked Coating Atop a Viscous or Elastic Base
• Photopolymerization and Structure Formation of Methacrylic Acid Based Hydrogels in Water/Ethanol Mixture
• Effects of Polymers and Asphaltenes on the Structure and Deposition Behavior of Waxy Gels
• Reversible Gelation of Polyethylenimine Solutions Using $CO_2$
• Structure, Property and Cure Kinetics of Thermosetting Copolymers

### Supramolecular Assembly of Inorganic Materials I
***Marriott San Francisco, Yerba Buena Ballroom 4***
• Self-Assembly of Nanoparticles at the Liquid-Liquid Interface
• Nanoporous Array-Based Inorganic Materials Via Molecular Self-Assembly Templated Processing

• Ternary Phase Diagram of Cationic and Maltoside Surfactants in Water, and Its Use for Predictive Synthesis of Ordered Mesoporous Silica
• Two-Stage Diatom Cell Culture for the Supramolecular Assembly of Silicon-Germanium Oxides Ordered at the Submicron and Nanoscales
• Dual-Layer Material Deposition on Tobacco Mosaic Virus
• One Pot Synthesis of Ordered Biphasic Mesoporous Silica with 2d Hexagonal and Mesh Structure and Its Use for Controlled Deposition of Metal Oxides

**Sustainability**
***Hilton San Francisco, Union Square 23***
• Benchmarking the Integration of Sustainability into Engineering Curricula at Us Institutions of Higher Education
• Graduate Education in Sustainability for Engineering and the Social Sciences: an NSF-Sponsored Intercampus Program
• A Global Perspective for Sustainable Design: New Opportunities for Deep Fried Sewage and Pureed Kelp
• Undergraduate Research- Use of Tga to Characterize Sludge Drying
• Bio-Oil Production from Algae Grown on Dairy Anaerobic Digestion Effluent: an Independent Senior Design Project

**THURSDAY, 16 NOVEMBER 2006**
***11:15 AM - 12:15 PM***
**Special Lecture: Environmental Change**
***Hilton San Francisco, Grand Ballroom A***
• Sound Science for Sound Decisions

**THURSDAY, 16 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**(22c) Nanowires I: Synthesis**
***Hilton San Francisco, Mason***
• Nanocrystal-Mediated Crystallization of Silicon and Germanium Nanowires in Organic Solvents: the Role of Catalysis and Solid-Phase Seeding
• Synthesis of Silicon-Germanium Alloy Nanowires Using Vapor-Liquid-Solid Method
• Fabrication of Double-Gyroid Structure Nanowire Arrays
• Template Synthesis of Gold/Conducting Polymer Composite Nanowires
• Fabrication of Novel Nanostructures Using Ordered Porous Templates
• Oriented Growth of Gan Nanowire Using Patterned Substrates

**Advanced Materials and Nanotechnology in Water Treatment, Purification and Desalination**
***Hilton San Francisco, Grand Ballroom A***
• Effects of Tio$^2$ Nanostructure and Various Ceramic Supports in Photocatalytic Membranes for Water Treatment
• Selective Metal Ion Binding with Inorganic and Organic Nanoparticles
• Adsorption of Acid Dye in Aqueous Solution by Mesoporous Carbons
• Mechanisms and Control of Irreversible Fouling in Commercial and Nano-Structured RO/Nf Membranes
• Electrocoagulation Mechanism for Cod Removal
• Design of a Fluidized Bed Biological Reactor for Reduced and Microgravity Operation

**Advances in Aqueous-Based Processes for Metals Separation and Purification**
***Hilton San Francisco, Union Square 13***
• A Reprocessing Plant for the USA Based on Proven Technologies Enhanced to Meet the Goals of the Global Nuclear Energy Partnership
• Ionic Liquids as Extraction Solvents: Current Status and Future Directions
• Lab-Scale Demonstration of the Urex+1a Process Using Spent Nuclear Fuel
• Practical Actinide Partitioning
• Separation of Uranium from Fission Products in Spent Nuclear Fuel Using Aqueous Hydrogen Peroxide-Carbonate Solutions
• Washing Savannah River Site Sludge with a Rotary Filter

**Advances in Drug Delivery II**
***Hilton San Francisco, Sutter***
• Probing and Modeling Spatial Distributions of Particulate Vaccines at the Respiratory Tract
• Pressurized Metered-Dose Inhaler Formulations for the Systemic Delivery of Biomolecule
• Inhaling Cationic Aerosols to Mitigate the Spread of Infectious Disease
• Extract of Pine Cones Augments Tumor Response to Electrochemotherapy
• Polymeric Nanogels as Potential Anti-Cancer Drugs
• Tissue Plasminogen Activator Carrying Worm Micelles as Prophylactic Fibrinolytic Agents
• Controlled Delivery of Paclitaxel from Electrohydrodynamically Atomized Microparticles and from Micro-Porous Foams for the Post-Surgical Treatment of Glioblastoma Multiform
• Spray Drying Cellular Material

**Advances in Porous Inorganic Materials I**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• The Formation of Solvent-Induced Porosity in Thin Hydrogen Silsesquioxane Films Via the Use of Co-Solvent Organic Mixtures as Gelation Agents and Pore Generators
• SBA-15/Zeolite Composites by Solid Phase Crystallization and Carbon Templating
• Controlling Zeolite Crystal Morphology Using Oil/Water/Surfactant Mixtures
• Mesoporous Calcium Phosphate Nanorods
• Mesoporous Carbon Nanocapsules from Enzymatically Polymerized Polyphenols Confined in Silica Aerosol Particles
• Investigation of the Formation Mechanism of Single Walled Aluminogermanate Nanotubes
• In Situ Saxs/Waxs of Zeolite Synthesis Using Microwave Heating

**Advances in Protein Structure, Function, Analysis and Stability - II**
***Hilton San Francisco, Powell***
• Structure and Aggregation in a Simple Helix-Forming Polymer
• Computer Simulation of Protein Aggregation Kinetics Using an Intermediate Resolution Model
• Smart Polymer Enhanced Protein Refolding: Molecular Dynamic Simulation and Experimental Validation
• Structure, Stability and Formation of the Nucleus in Polyglutamine Aggregation
• Salt Effects on the Aggregation of Amyloid Fibril Forming Proteins
• Molecular Insights into Interactions between Misfolded Proteins and Application to Prion Transmission Barriers
• Protein Aggregation at Interfaces – Lipid Induced Amyloid-Beta Fibril Formation

**Alternative Fuels and Enabling Technologies I**
***Hilton San Francisco, Imperial A***
• Aldehyde Formation in Spark Ignition Engines
• Engine Emissions and Performance Characterization for Variable Gasoline-Ethanol Blend Concentration
• Kinetic Model for Gasoline Gum Formation during Storage under Use Conditions in Vehicle Engine
• A Carbon Dioxide Ssitka Study of Carbonate Formation on Gamma-Alumina Employing a Novel Transmission Ftir-MS System
• Investigation of the Reverse Water-Gas Shift Reaction on a Cu/Gamma-Al2o3 Catalyst Employing a Newly Constructed Ssitka System Employing Transmission Ftir-MS Detection

**Biological Conversions and Processes for Renewable Feedstocks I**
***Hilton San Francisco, Continental 6***
• Alternative Routes for Conversion of Biomass to Fuels and Chemicals
• Flexible Biorefinery for Producing Value-Added Streams: Evaluation of the Cellulose Stream as a Source of Sugars and Pulp
• The Effects of AFEX Pretreatment on the Fermentability of Lignocellulosic Hydrolysates Using *Escherichia Coli* KO11
• Impact of Culture Nutrition on the Tolerance of Furan Inhibitors and the Conversion of High Xylose Concentrations to Ethanol by *Pichia Stipitis* Nrrl Y-7124
• Ethanol Production from Xylose by Ethanol Resistant Derivatives of *Escherichia Coli* FBR5 under Batch and Fed-Batch Conditions
• Bioethanol Production from Cellulosic Materials by Cell Surface Engineered Yeast Strains
• Reaching High Substrate Loading in the Lignocellulose to Ethanol Process; Effects of Multiple Batches of Substrate Loading on Enzymatic Hydrolysis and Viscosity of Pretreated Barley Straw

**Biomaterials for Drug Delivery I**
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Photocured Hyaluronic Acid Films Functionalized with Cyclodextrin
• Molecular Analysis of Interpolymer Complexing Hydrogels Based on Poly(Methacrylic Acid) and Poly(*n*-Vinyl Pyrrolidone) as Carriers for Protein Delivery by Transmucosal Transport
• Hydrogel-Nanofiber Composite Systems for Drug Delivery— Kinetics of Fiber Hydrolysis and Drug Release
• Gene Delivery from Polymer Scaffolds for Angiogenesis
• Development and Evaluation of Minocycline/Rifampicin-Impregnated Silicone Catheters: a Potential Tool for the Treatment of Csf Shunt Infection
• Release of DNA from Intravascular Stents Coated with Ultrathin Multilayered Polyelectrolyte Films
• Biomaterials Based on Polyethylene Glycol-Dihydroxyacetone Block Copolymers

**Biomems and Microfluidics: Proteome Analysis**
***Hilton San Francisco, Union Square 19 & 20***
• Fabrication, Optimization, and Application of a Micro-Free Flow Electrophoresis Microfluidic Chip
• Microfluidic Chemical Cytometry Based on Modulation of Local Field Strength
• A Self-Contained Solid-State Micro-Valve for Electrokinetic Separations in a Networked Microfluidic Chip
• Effect of Channel Morphology on Electrophoretic Transport
• Two Dimensional Simulation of Nonlinear Electrophoresis of Proteins and Experimental Demonstration in a Microfluidic Chip
• Rapid Assessment of Markers in Serum Using Biomems ELISA

**Biomimetics III: Cell-Material Interactions**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Effect of Adhesion Peptide Incorporation in Poly (L-Lactic Acid) Scaffolds on the Osteoblastic Differentiation of Mesemchymal Stem Cells under Conditions of Flow Perfusion
• Osteonectin-Derived Peptide Significantly Affects Modulus of Apatite/Hydrogel Composites
• Insect Cuticle as a Motif for Crosslinked Biomimetic Materials
• Engineering of PHßV Microspheres of Enhanced Biomolecular Recognition by Hep3ß Liver Cells in the Presence of Biomimetic Collagen
• Chemical and Topographical Modification to Polydimethylsiloxane Surfaces Affect Growth and Adhesion of CaCo-2 Cells
• Role of MW of Negatively-Charged Polymer on

Cell Colonization in 3-D Matrices
• The Use of Polymers in the Development of an Ex Vivo Three-Dimensional (3-D) Model of Human Acute Myeloid Leukemia (AML)

### Cape-Open Unit Operations: Development and Usage
***Hilton San Francisco, Union Square 24***
• Cape-Open Integration for Advanced Process Engineering Co-Simulation
• Prosimplus: New Cape-Open Capabilities
• Heat Exchanger Rating Using Cape-Open in a Process Modeling Environment
• Ipsepro: a Cape-Open Unit Plug for Advanced Power Plant Equipment Modeling
• New Cape-Open Unit Operations Socket in Equation-Oriented Process Modeling Environment
• Development of Cape-Open Unit Operations for Advanced Power Systems Modeling
• Hybrid Solution Approach – Cape-Open in Unisim Thermo Unit-Operations

### Catalysis for Pharmaceuticals and Fine Chemicals
***Hilton San Francisco, Franciscan C***
• Biocatalysis of Beta-Lactam Antibiotics
• Catalytic Hydrogenation Reactions in Fine Chemicals: Applications in Tandem Synthesis and Relevant Reaction Engineering Issues
• Copper Chloride - Assisted Oxidative Cyclization of Amidrazones Derivatives
• Development of Heterogeneous Group 4 Metallocenes: Synthesis, Application and Molecular Modeling
• Stereoselective Synthesis of Alicylic Amines
• Understanding the Enhanced Enantioselectivity during Hydrogenation Using a Supported Ruthenium Mab Complex

### Catalytic Conversion of Renewable Resources to Synthesis Gases and Pyrolysis Oils
***Hilton San Francisco, Continental 9***
• Technoeconomic Comparison of Indirectly Heated and Directly Heated Gasification Processes for Making Mixed Alcohols Via Catalytic Upgrading of Synthesis Gas

• Gas Cleanup Technologies Suitable for Biomass Gasification to Liquid Fuels
• Upgrading Producer Gas from Biomass Gasification to Produce High Purity Hydrogen
• Production of Clean Synthetic Gas from Biomass Using a Downdraft Gasifier
• Biomass Gasification with Nickel Oxide/Olivine Catalysts in Fluidized Bed Gasifier
• Production of Synthesis Gas and/or Hydrogen from Biomass Via Fast-Pyrolysis and Reforming Process
• Stability Assessment of Wood and Bark Derived Bio-Fuels

### Collaborative Projects with Industry
***Hilton San Francisco, Union Square 21***
• Ten Years of Industrially Sponsored Capstone Design Projects
• Challenges of Implementing a Joint Industrial - Academic Research Project as Part of a Non-Traditional Industrial PhD. Dissertation
• Undergraduate Academic Credit through on-Site Industrial Experiences: a Problem or an Opportunity?
• Academic-Industrial-Government Collaboration through the Engineering Clinic Program at Rowan University
• The Experimental Prototype: Critical Thinking and Real-World Problem Solving in Engineering Education
• Industrial Collaboration in the Capstone Design Courses: Experiences at Oklahoma State University

### Complex and Networked Systems II
***Hilton San Francisco, Van Ness***
• Finite Element & Finite Difference Methods for Cardiac Propagation
• Distributed Model Predictive Control of a Benchmark Chemical Plant
• Fault-Tolerant Control of Process Systems Using Robust Model Predictive Control
• System Level Component Models for Electrochemical Power Sources in Hybrid Environments
• Complex Supply Chain Networks
• A Two-Dimensional Dynamic Model for a Tubular Solid Oxide Fuel Cell ( SOFC)

### Computational Biology: Proteins and DNA
***Hilton San Francisco, Union Square 17 & 18***
• Role of Histone Tails and Linker Histone in Chromatin Folding
• MD(T, F) and Experimental Studies on the Thermomechanical Stability of Three-Helix Bundle Repeats
• Molecular Dynamics Simulations to Guide the Design of Peptide Antibiotics
• Insights into a Model Peptide System - a Polarizable Force Field Molecular Simulation Study
• Physics-Based Protein Structure Prediction by Zipping and Assembly
• An Improved Coarse Grain Model of DNA and Applications
• Modulating the DNA Affinity of Elk-1 with Computationally Selected Mutations
• Molecular Dynamics of DNA Translocation through Nanoelectrode Gaps

### Desalination Processes - II
***Hilton San Francisco, Plaza A***
• Mixed Mineral Scale Formation in Low-Pressure Reverse Osmosis Membrane
• Prevention of Precipitation Fouling in RO by Reverse Flow Operation
• Coupled Effects of Salt Concentration Polarization and Colloidal Deposition on the Performance of Reverse Osmosis Membranes
• Modeling and Shortcut Calculation for Efficient VMD with Crossflow Modules
• ETV Testing of Expeditionary Water Purification Equipment - Wastewater Challenge

### Design & Synthesis of Sensor Systems
***Hilton San Francisco, Union Square 25***
• Sensor Network Design Via Observability Analysis and Principal Component Analysis
• Computing Sensor Locations for Nonlinear Systems under the Influence of Disturbances
• Constraints Driven Optimal Actuation Policies for Distributed Parameter Systems with Collocated Actuators and Sensors
• New Sensor Network Design Formulation Maximizing Economic Value of Accuracy
• Design of a Diagnosis-Based Sensor Network
• Covariance Based Hardware Selection for Infinite Dimensional Systems

### Drug Delivery (I)
***Hilton San Francisco, Yosemite A***
• Design of Targeted Nanocarriers for Optimal Drug Delivery to Stressed Endothelium: a Multiscale Modeling Approach
• Comparative Analysis of the Uptake and Intracellular Fate of Nanoparticles in Different Epithelial Cell Types
• Efficient Sirna Delivery with Acetylated Polyethylenimine
• Biodegradable Spray Dried Microspheres and Discs Delivering Paclitaxel and Etanidazole for the Treatment of Giloma: an in Vivo Subcutaneous Study
• Coated Microneedles for Transdermal Drug Delivery
• A Biodegradable Fiber for Controlled Delivery of Therapeutics to the Eye
• Drug Elimination Kinetics in the Eye after Subconjunctival Delivery
• Incorporation of Statins in a Perivascular Polymeric Drug Delivery Device for the Inhibition of Intimal Hyperplasia

### Environmental and Industrial Sensors
***Hilton San Francisco, Union Square 1 & 2***
• Cell-Based, Non-Invasive Sensing of Inhalation Health Hazards
• Sensor Material Selection and Response Modeling for the Jpl Electronic Nose Using Molecular Modeling Tools
• Zeolite Thin Film-Based Fiber Intrinsic Fabry-Perot Interferometric Sensor for Detection of Dissolved Organics and Ions in Water
• Chelator-Doped Conducting Polymer Thin Films for Heavy Metal Ion Detection
• A Colorimetric Sensor Array for the Detection of Toxic Industry Chemical (Tics)
• Electrostatic Tomography for Process Measurement and Control
• A Study on Ect Sensors Applied to Conductive Media
• Coupled Resonances on the QCM and the Lumped Equivalent Model

### Environmental Fate and Transport Processes II
***Hilton San Francisco, Union Square 15 & 16***
• Emission of Polynuclear Aromatic Hydrocarbons from Contaminated Sediments
• Modeling Free-Radical Reactions for Hydrogen Peroxide/Ultraviolet (HP/Uv) Oxidation: Optimizing Membrane Process Efficiencies in Drinking Water Treatment
• Removal of MTBE from Groundwater Using Biosparging
• Predicting Bioaccumulation in Dynamic Food Webs: Ontogeny, Seasonality and Invasional Successions
• In-Situ Measurement of Rhizosphere Degradation Kinetics

### Fuel Cell Membranes I
***Hilton San Francisco, Continental 2***
• Nafion/Acid Functionalized Zeolite Beta Nanocomposite Membrane for High Temperature PEMFCs
• Novel Sulfonated Polyimide Copolymers for High Temperature Proton-Exchange Membrane Fuel Cells
• Modified Nafion as the Membrane Material for Direct Methanol Fuel Cells
• Nafion® Blend Membranes for the Direct Methanol Fuel Cell
• Near Net-Shape Fabrication of Nafion® Membranes for Fuel Cell Applications
• Polyelectrolyte Multilayer Membranes for the Preparation of Proton Exchange Membranes in Direct Methanol Fuel Cells

### Fuel Cell Technology IV
***Hilton San Francisco, Continental 7***
• Comprehensive Modeling of a Microbial Fuel Cell
• Catalytic Activities of Mixed Conductive Bi2ti0.1v0.9o5.45 for $H_2$/Methanol Oxidation in Acid Aqueous Solution
• Design Considerations for PEMFC Cathode Air Filters
• Performance Characterization of Supported Palladium Catalysts for Direct Formic Acid Fuel Cells
• Residence Time Distribution of Anode Impurity Pulses in a 47 Cell PEM Stack
• A Pseudo-3d Simulation Model for Proton Exchange Membrane Fuel Cells
• Observer Design for SOFC Cold Start

### Fuel Cells: Fuel Processing I
***Hilton San Francisco, Continental 3***
• Integrated Autothermal Micromembrane Fuel Processor for Fuel Cell Application
• Hydrogen Production from Jet Fuel
• Modeling the Transient Response of Heat Exchange Reformers
• Development of a Novel Flexible Fuel Reformer with Sulfur Tolerant Catalyst
• Hydrogen Generation by Partial Oxidation of Propane over Tio2- $Al_2O_3$ Supports

### Genomic Approaches to Systems Biology I
***Hilton San Francisco, Imperial B***
• Gibbs Sampling for Transcription Network Verification Using Gene Expression and Chip-Chip Data
• Bioinformatic Profiling of Short Term Liver Response to Thermal Injury
• Immune Signaling Gene Expression Exhibits Multiple Temporal Patterns in Influenza Infected Mouse Lung
• Genomics for the Validation of in Vitro Blood-Brain Barrier Models
• Defective Virus Genomes: toward Mechanisms of Emergence and Growth
• An Analysis of the Dose-Dependent Global Transcriptional Response of *Saccharomyces Cerevisiae* to Multiple DNA-Damaging Agents

### Global Sustainability Strategies and Stories
***Hilton San Francisco, Continental 5***
• Life Cycle Assessment of Honda Accord Hybrid Vehicles
• Environmental Benefits of Polymers – from Classical Polymers to Bio-Based Materials
• A Cradle to Gate Life Cycle Analysis of the Biopolymer Polylactic Acid: Looking beyond Global Warming and Fossil Fuel Use
• Estimating the Potential Economic Impact of Greenhouse Gas Costs on the Chemical Industry
• Evolution and Analysis of Phosphorus Metabolism in China
• Reduced Data Techniques for Cleaner Production Evaluation for Surface Treatment Plants

### Impact of Process Intensification on Process Design
***Hilton San Francisco, Union Square 23***
• Systematic Retrofit Design of Batch Processes Using an Indicator and Model Based Framework
• Comparison of Enzymatic and Chemical Epoxidation of Oleic Acid Esters in a Fluidized Bed Reactor
• Experimental Study of the Process for Making Tackifier Dispersions Used in Pressure-Sensitive Adhesives
• Experimental Verification of Hydrodynamic Multiplicity in an Industrial Trickle Bed Reactor
• Gas-Liquid Mass Transfer in Slug Flow through Narrow Channels
• Experimental and Theoretical Investigation of Photopolymerization Using a Narrow Channel Reactor
• Thermodynamic and Graphical Analysis of Integrated Processes: a Reactive Distillation Process Case Study

### Microreaction Engineering I
***Hilton San Francisco, Franciscan B***
• Conversion of Glucose to Hydrogen Gas by Supercritical Water within a Microchannel Reactor
• Thermal Management in Devices for Portable Hydrogen Generation
• Catalytic Microcombustors with Integrated Thermoelectric Elements for Portable Power Production
• Validation of CFD Models for a Microscale Confined Impinging-Jet Reactor Using Micro-Piv and Reactive LiF
• Confinement Effects in Catalytic Microchannel Reactors: Turning a Catalyst into a Reaction Inhibitor
• Catalyst Coating Studies in Multi-Channeled Structures for Steam Reforming of Methanol

### Molecular Modeling of Fuel Cells and Electrochemical Systems II
***Hilton San Francisco, Union Square 3 & 4***
• Molecular Dynamics Simulations of Proton Solvation and Transport in Polymer Electrolyte Membranes
• Molecular Studies of the Structural Properties of Hydrogen Gas in Liquid Water
• Lithium Transport in Binary and Single Ion Conductor Liquid, Gel and Polymer Electrolytes
• Simulating the Electrochemical Double Layer Using Charge Dynamics
• Theoretical Investigations of Modified Active Site Models for Fe-Only Hydrogenases
• Multi-Paradigm Simulations toward the Design of Improved Fuel Cell Catalysts and Membranes
• A Molecular Dynamics Study of Nafion Polyelectrolyte Membrane and the Aqueous Phase Structure for Proton Transport
• Molecular Dynamics Study on Hydrated Water-Soluble Dendrimer-Grafted Polymer Membrane for PEMFC

### Multiphase Mixing I: Gas-Liquid Mixing
***Hilton San Francisco, California Room***
• Stirred Tanks: a Physical Explanation for the Exponents of Classical Empirical Mass Transfer Equations
• Characterization of the Gas Dispersion Capabilities of the Bt-6 Impeller
• On-Line Measurement and Power Consumption Simulation on Gas-Liquid Agitated Systems
• Simulating Gas-Liquid Flow in Aerated Stirred Bioreactors Based on CFD-PBM Model
• Effect of Scale on the Hydrodynamics of Low L/D Internal Gaslift Loop Reactor for Anaerobic Digester Applications
• Gas Holdup in Bubble Columns with and without Vibrating Internals
• Gas-Liquid Flow in a Rectangular Partially Aerated Bubble Column: Combined Effect of Aspect Ratio and Superficial Gas Velocity

### Nanoscale Structure in Polymers II: Nanostructured Polymeric Materials
***Hilton San Francisco, Continental 4***
• Confinement Effects on the Crystallization of Perfectly Linear Polyethylene
• Crystallization and Orientation Studies in SWNT Based Nanocomposites
• Equilibrium Dynamics of a Polymer Bicontinuous Microemulsion
• Design of Polymer Blends with Nanoscale Dispersed Phases Using Melt Processing and Solid-State Shear Pulverization
• Anisotropic Swelling in Polymer Nanostructures near a Rigid Substrate
• Effect of Cylindrical Confinement on Self-Assembly of Block Copolymers within Co-Axial Electrospun Fibers
• Functional Nanofibers of Associative Polymers Via Electrospinning
• Using Cross-Section Surfaces of Polymeric Multilayer Films as a Nanopatterning Template

### Nanostructured Organic/Inorganic Hybrid Materials
***Marriott San Francisco, Yerba Buena Ballroom 5***
• Dendrimer/Oms Hybrid Materials
• Molecular Design of Aminopropyl-Functionalized Silica: Probing Amine Separation and Surface Functionalization Mechanism
• Synthesis and Characterization of Bifunctional Silica Imprinted Surfaces
• Directed Growth of Surfactant-Silica Nanostructured Hybrid Materials through Electroosmotic Flow
• MC Simulations of Self-Assembling Amphiphilic Systems with Terminal or Bridging Organosilica Precursors
• Ultra-High Strength Clay-Polymer Layered Nanocomposites: Artificial Nanostructured Nacre a Step Further
• Synthesis and Morphology Characterization of Mesoporous Silica/Single Wall Carbon Nanotubes Composites

### Novel Reactor Design
***Hilton San Francisco, Franciscan A***
• Microwave Synthesis Engineering - the Effect of Frequency and Power Delivery
• Sonochemical Removal of Nitric Oxide from Flue Gases
• Production of Oxygenated Hydrocarbons by Plasma-Assisted Reforming of Diesel Fuel
• Design and Characterization of a Novel Chemical Vapor Deposition Reactor to Synthesize Nanoscale Structures
• Catalytic Hot Oxygen Reactor
• Comparison of the Performance of a Reverse Flow Reactor and Networks of Non-Stationary Catalytic Reactors for Catalytic Combustion of Methane in Lean Mixtures
• Heterogeneous–Homogeneous Catalytic Partial Oxidations Investigated by Molecular Beam Mass Spectrometry
• Design of Nonisothermal Plug Flow Reactor Using Neons

### Planning
***Hilton San Francisco, Union Square 5 & 6***
• Simultaneous Optimization Approach for Feedstock Selection and Operating Conditions for an Olefins-Aromatics Planning Problem
• Optimal Integration of Planning and Scheduling for Parallel Multi-Product Batch Reactors
• Optimal Planning Strategy for the Supply Chains of Olefins and Aromatics under Demand Uncertainties
• Process Cost Modeling and Production Planning for Petrochemical Industries under Uncertainties
• A Process Attainable Region Approach for Production Planning
• Strategic Planning in the Pulp and Paper Industry under Uncertain Conditions – a Fuzzy Optimization Approach

### Polymerization Reaction Engineering, Kinetics, and Catalysis I
***Marriott San Francisco, Yerba Buena Ballroom 6***
• Reaction Mechanisms and Kinetic Modeling of Ternary Thiol-Vinyl Photopolymerizations
• Ftir Imaging for Spatial Analysis of Polymerizations
• Kinetic Characterization of Surface-Initiated Photoiniferter-Mediated Photopolymerization in Presence of Tetraethylthiuram Disulfide
• Mechanistic Modeling of Nitroxide-Mediated Controlled Radical Polymerization
• Carbon Black Acts as Catalyst in Making Amphiphilic LPNS Based on Pulverized Rubber Particles
• Ru-Catalyzed Ring-Opening Metathesis Polymerization Route to Narrow-Distribution Polyethylene
• Systematic Kinetic Modeling and Optimization of Polycondensation Reactions

### Removal and Detection of Emerging Contaminants
***Hilton San Francisco, Plaza B***
• Overview of EPA's Water Security Decontamination Research
• Pilot-Scale Evaluation of Various Approaches for the Decontamination of Drinking Water Distribution Systems
• Contamination and Decontamination of Building Plumbing Systems
• Drinking Water Decontamination with Immobilized Enzymes
• Viability of Nanofiltration and Reverse Osmosis in Removing Emerging Trace Organic Contaminants
• Molecularly Imprinted Polymers for Estrogenic Pollutants Removal

### Simulation and Control of Multiscale Systems II
***Hilton San Francisco, Taylor***
• Equation-Free and Equation-Assisted Computation for Spatially Distributed Multiscale Models
• A Multi-Physics Coupling Technique That Preserves Nonlinear Globalization Strategies
• Model Reduction and Optimal Control for the Autothermal Reforming (Atr) Reactor
• Construction of Nonlinear Stochastic PDES for Nonlinear Feedback Control of Surface Roughness: Application to a Sputtering Process
• A Hybrid Meta Density Functional Theory Study

Examining the Association Patterns in $(HF)_n$-$(H_2O)_M$ Clusters
• Efficient Multiscale Dynamic Optimization of Thin-Film Growth Via Model-Reduction: Application to Gaas Epitaxial Growth

**Site Assessment and Remediation - II**
***Hilton San Francisco, Lombard***
• Assessment of Buoyancy Effect on EK Removal Efficiency and Its Implication for *in-Situ* Applications
• Laboratory Scale Treatment of CCA Contaminated Wood Waste
• Electrokinetic Treatment of Mercury Contaminated Soil at the Mercury Refining Company Superfund Site
• Electro-Kinetic Enhanced Air Sparging Soil Remediation Process under Non-Ideal Conditions
• The Exploration of Conditions in Which Chlorinated Benzenes Are Degraded by Zero-Valent Iron
• Phenanthrene Removal on a Permeable Reactive Biobarrier Treated with Beijerinckia Indica

**Solids Handling and Processing**
***Hilton San Francisco, Franciscan D***
• Flowability Modification of Fine Powders by Plasma Enhanced Chemical Vapor Deposition
• Characterizing the Effect of Substrate Surface Roughness on Particle-Wall Interaction by Airflow Method
• Correlating Density Measurements to Flow Behavior of Cohesive Granular Materials
• Effect of Ambient Temperature on Solids Induced Loads on the Walls of Silos
• Investigations of Intra-Tablet Coating Variability in a Side-Vented Pan Coater Via Digital Video Analysis
• Inter-Tablet Coating Variability in a Horizontal Axis Pan Coater
• Flow Transitions in a Model High Shear Granulator
• Investigation of Particle Electrification in Mixers - Effect of Particle Size, Mixer Type, and Rotation Speed

**Surfaces and Interfaces**
***Hilton San Francisco, Continental 1***
• The Assembly of Conjugated Dithiols on Gold and Gallium Arsenide
• Deposition of Reactive Procion Dyes in Layer-by-Layer Films for Second Order Nonlinear Optical Materials
• Probing Organic Field Effect Transistors (Ofets) *in-Situ* Using SFG
• Orientational Dynamics of Polydiacetylene Monolayers
• Surface Chemistry of Carbon Overcoats for Magnetic Data Storage

**Sustainability in Product Design**
***Hilton San Francisco, Union Square 22***
• Inertial Separation of Airborne Nanoparticles with Fibrous Filters
• Molecular Simulation Study of Temperature, Pressure and Diameter Effects on Dynamic Properties of Carbon Dioxide Confined in Carbon Nanotube
• Tracing the Path to Success in Industrial Catalyst Development
• $K_2CO_3$ Supported Sodalite: Control of Carbon Nanoparticles Emission for the Rectification of Air Contaminants
• Striking Gold in Catalyst Development
• Development of a Process for Manufacturing Industrially Important Chemical Products from Sustainable, Bio-Based Glycerol
• The Industrial Metabolism of Chlorine in China

**Systems Biotechnology**
***Hilton San Francisco, Yosemite B***
• A Stochastic Model of E. Coli Ai-2 Quorum Sensing Circuit Reveals Alternative Synthesis Pathways
• Exploiting Transcriptional Patterns of Antibiotic Activity for Treatment Optimization and Development
• Transcriptomic Deduction of *Escherichia coli's* Reactive Nitrogen Oxide Species Sensing Circuits
• Signaling Pathways Affecting Sporulation and Stationary Phase Phenomena in Clostridium Acetobutylicum
• Transcriptional Regulation Underlying the Central Nervous System Response to Acute Hypertension
• Comparative Transcriptome Analysis of Stem Cell Populations Expressing Varying Levels of the Transcription Factor Oct-4
• Comprehensive Analysis of the Gluconeogenesis Pathways through the Combined Use of Multiple Isotopic Tracers

**Tissue Engineering: Stem Cells in Tissue Engineering (I)**
***Hilton San Francisco, Yosemite C***
• Assembly of Embryonic Stem Cell/Scaffold Three-Dimensional Constructs Using Carbon Dioxide Assisted Polymer Fusion
• Engineering/Controlling Microenvironments for Cardiovascular Differentiation of Human Embryonic Stem Cells
• Adeno-Associated Virus-Mediated Gene Delivery to Adult and Embryonic Stem Cells
• Engineering of Implantable, Bi-Layered Tissue-Engineered Blood Vessels from Adult Bone Marrow Stem Cells
• Isolation and Differentiation of Porcine Progenitor Cells into Endothelial-like Cells for Vascular Tissue Engineering
• Integrin Linked Kinase Production Prevents Anoikis in Human Mesenchymal Stem Cells
• Stem Cell Engineering: from 2d to 3d
• Satellite Cell Modeling by a Population Balance Incorporating Terms for Contact Inhibition

**Transport in Fluidized Systems**
***Hilton San Francisco, Union Square 14***
• Entrainment into a Submerged Jet within a Fluidized Bed
• Lower Order Modeling of Cold Mockup Spouted Bed for Nuclear Fuel Particle Coating as Well as Experimental Results for Spout Height Correlations
• Solids Fraction Measurement with a Reflective Fiber Optic Probe
• Mass Transfer Coefficient for Drying of Moist Particulate in Bubbling Fluidized Bed
• Understanding Streaming Flow in Deep Fluidized Beds
• Removal of Residual Monomers and Solvents from Granular Polymers in Fluidized Beds; Experimental • Methods of Measurement of Diffusivity and Solubility Parameters for Design and Troubleshooting
• Tudy Characteristics of Complicated Flow Field in Bubbling Fluidized Bed by CFD

**Transport Processes in Energy Systems**
***Hilton San Francisco, Continental 8***
• Enhanced Heat Removal Due to Pulsatile Flows
• Evaluation of the Boundary Conditions in CFD Modeling of Heat Transfer in the 3d Chevron Type Plate Heat Exchanger
• Experiments and Simulations for Evaluating Relative Flow of Gas and Water in Tight Gas Reservoirs
• Utilizing the "Cool" in LNG
• Importance of Soret Transport and Heterogeneous Chemical Reactions in the Deposition of Trace Heavy Metals from Combustion Gases
• Soret Effects on Gaseous Diffusion Flame Temperatures and Positions
• Monitoring Yielding Condition of a Viscoelastic Waxy Oil Gel
• Natural Convection Effects on Freezing in Finned Rectangular Containers
• Studies on Ionic Mass Transfer with Orifice–Disc Turbulence Promoter
• Utilizing the "Cool" in Liquefied Natural Gas

## THURSDAY, 16 NOVEMBER 2006

***3:15 PM - 5:45 PM***

**(22b) Micro- and Nanodevices for Targeted Therapeutics II**
***Hilton San Francisco, Union Square 1 & 2***
• Medical Micro- and Nano-Technology: Case Studies in Transdermal Drug Delivery
• Needle-Free Transdermal Drug Delivery Using Pulsed Piezoelectric Microjets
• Multiphasic Polymer Nanocolloids with Potential Use for Drug Targeting
• In Vitro Ultrasound-Mediated Leakage from Phospholipid Vesicles
• Wireless Induction Heating of Stratum Corneum for Transdermal Drug Delivery
• Microfluidic Probes for Tracer Studies of Convective Transport in the Brain

**(22c) Nanowires II: Modeling and Fundamental Properties of Nanowires**
***Hilton San Francisco, Mason***
• Electrodeposition of Bismuth Telluride Nanowires for Thermoelectric Applications: Synthesis, Characterization, and Properties
• Synthesis and Raman Spectroscopy of Sic Nanowires
• Molecular Dynamics and Density Functional Theory Studies on the Formation of Ultrathin Gold Nanowires in Vacuum and in Organic Solvents
• Molecular Dynamics Simulation Study of Transition Metal Nanowires under Uniaxial Tension: Temperature and Strain Rate Effects
• Sub-Picosecond to Nanosecond Carrier Dynamics in Zinc Oxide Nanowires and Films Measured by Time-Resolved Terahertz Spectroscopy
• First Principles Studies of the Structural and Opto-Electronic Properties of Silicon Nanowires
• Molecular Spring Assemblies from Nanowires

**Advanced Methods and Concepts in Water Treatment and Production**
***Hilton San Francisco, Plaza A***
• Biological Treatment of Perchlorate by Autotrophic Organisms Attached to Zero-Valent Iron
• Combinative Sonophotochemical and Sonophotocatalytic Oxidation Processes for the Treatment of Pollutants in Water: an Overview and Future Research Needs
• A New Benign Separation System: Hydrophilic Ionic Liquids-Glucose-Water
• Liquid Phase Nitrate Reduction
• Heavy Metals Removal from Wastewater by Magnetic Field-Magnetotactic Bacteria Technology
• The Prospect of Using LNG Regasification as a Heat Sink for Seawater Desalination

**Advances in Computational Approaches to Systems Biology**
***Hilton San Francisco, Union Square 25***
• A High Resolution Side Chain Centroid Based Distance Dependent Force Field - Effect of Protein Side Chain Interactions
• Circadian Phase Entrainment Via Nonlinear Model Predictive Control
• Sensitivity Analysis-Based Approach for Identifying Key Steps in Cell Signaling for Hepatocytes Stimulated by Il-6
• Parameter Estimation for Stochastic Models: Application to Genetic Networks
• Mocat: an Algorithm for Learning Boolean Functions from Noisy Data and Its Application to Learning Interacting Residues in a Protein
• Structural Analysis of Biological Regulatory Networks
• Balanced Metabolic Reaction Networks
• Equation-Free Analysis of Gene Regulatory Networks

**Advances in Porous Inorganic Materials II**
***Marriott San Francisco, Yerba Buena Ballroom 1***
• Aspects of a Novel Method for the Pore Size

Analysis of Thin Silica Films Based on Krypton Adsorption at Liquid Argon Temperature (87.3k)
• Zeolite a/ZSM-5 Hybrid Coating
• Dielectric Constant Measurement of Pure-Silica-Zeolite Fer Single Crystal by Time Domain Reflectometry (TDR)
• Dimensional Control of Single Walled Aluminosilicate and Aluminogermanate Nanotubes
• Synthesis and Application of Fluorocarbon Functionalized Mesoporous Silica
• Synthesis and Characterization of Functionalized Mesoporous Silica by Aerosol-Assisted Self-Assembly
• A New Method to Synthesize Micrometer-Sized Silica Spheres with Highly Ordered Mesostructure

### Algorithms, Applications, and Best Practices in Parallel and Grid Computing
***Hilton San Francisco, Taylor***
• A Parallel System for Describing and Analyzing Complex Chemical Kinetics
• Parallel Global Optimization for NLP and MINLP Programming Problems
• 3-D Compositional Streamline Reservoir Simulator – a Parallel Implementation
• Compositional Streamline Simulator with Gravity and Compressibility Effects
• High Fidelity, High Performance Simulation of Accidental Releases, Fires and Explosions in the Energy Industry
• Computationally Efficient Analysis of Large Array Ftir Data in Chemical Reaction Studies Using Distributed Computing Strategy

### Alternative Fuels and Enabling Technologies II
***Hilton San Francisco, Imperial A***
• Coal Gasification for the Production of Chemicals
• Production of a Biofuel from Sewage Sludge
• Production of Green Diesel through Catalytic Cracking of Phospholipids
• Exergy Analysis of a Gas to Liquid Process
• Transesterification, Modeling and Simulation of Batch Kinetics of Non-Edible Vegetable Oils for Biodiesel Production
• Transesterification Rates for Acid Catalyzed Methanolysis of Model Glycerides

### Biomaterial Product Design
***Hilton San Francisco, Union Square 22***
• Segmented Poly(Ester Urethane)Urea Elastomers with Biodegradable Hard and Soft Segments
• Fabrication and Characterization of Polymeric Surfaces for Bacteria Adhesion in Whole Cell Biosensor Using PECVD
• Improving Bioactive Glass from a Cellular Point of View
• Glass and Bioactive Glass Nanopowders by Flame Synthesis
• Influence of Surface Roughness and Hydrophobicity on Bacterial Adhesion and Colonization
• Biodynamic Test Instrument for Characterization of Tissues and Biomaterials
• Patterned Chemical Vapor Deposition Polymerization of Functionalized Poly-P-Xylylene for Spatial Control of Protein Adsorption and Cell Adhesion

### Biomaterials for Drug Delivery II
***Marriott San Francisco, Yerba Buena Ballroom 3***
• Engineering Shape of Drug Delivery Particles
• High Throughput Fabrication of Polymeric Microparticles
• Characterization of Anisotropic Biphasic Nanoparticles for Biomedical Applications
• Effects of Synthesis Methods on the Diffusion Coefficient of Proteinase K through Silica Nanoparticles
• Degradable Polymeric Hydrogels for Neurotrophin Elution from Implanted Prosthetic Devices
• Microfabricated Nanoporous Silicon Membranes for Drug Delivery Applications
• Plasminogen Activators as Prophylactic Fibrinolytics: Overcoming Free Protein Shortcomings

### Biomems and Microfluidics: Cell and Biomolecule Analysis
***Hilton San Francisco, Union Square 19 & 20***
• Electroporation of Mammalian Cells in a Microfluidic Channel with Geometric Variation
• Design and Fabrication of High-Throughput Microfluidic 3-Dimensional Cell Culture Systems
• On-Chip Aqueous Two-Phase Extraction for Protein Isolation from Cell Lysate
• A Neuron-Compatible Microfluidic Gradient Generator
• Three-Dimensional Assembly of Biomedical Micro/Nanodevices Containing Cells/Biomolecules Using Carbon Dioxide
• Biomems for Studying C. Elegans Olfaction Behavior
• Microelectrode-Based System for Cell Adhesion Detection and in Vivo Biofilm Monitoring

### Cape-Open Compliant Thermodynamic Components
***Hilton San Francisco, Union Square 24***
• An Assessment of the Computational Penalties Incurred by Using Cape Open Property Packages in Distillation Column Simulation
• Cape-Open Thermodynamic 1.1 Integration in Unisim Design - Advantages and Discussions
• Combined Thermodynamic Model Development and Cape-Open Implementation – an Industry Case Study
• Powering Process-Simulators with Predictive Cosmo-RS Thermodynamics
• Thermodynamic Utility – Importance and Potential Cape-Open Standard
• Use of a Cape-Open Thermodynamic Server in Legacy Codes

### Chemical Reactor Dynamics
***Hilton San Francisco, Franciscan A***
• Coupling Exothermic and Endothermic Reactions in Adiabatic Reactors
• Transversal Hot Zones in a Shallow Packed-Bed Reactor during Single or Multiple Reactions
• "Fan the Flame with Water". Current Ignition and Front Propagation in PEM Fuel Cells
• Enhancing Microburner Stability for Portable Power through Heat Recuperation
• Simulation of Three-Phase Spouted Bed Reactor for Solid Alkylation
• Oxidation of Hydrogen Sulfide in Coal Gases Producing Liquid Element Sulfur
• Modeling of $NO_x$ Storage and Reduction in Catalytic Monolith Reactors

### Computational Biology: Systems Modeling I
***Hilton San Francisco, Union Square 17 & 18***
• Computational Approaches for Prediction of Cross Reactivity in Human Protein Kinome
• Separating True Positive Residue Contacts from False Positive Ones in Proteins, Using Constrained Metropolis Monte Carlo Simulations
• Atomic Molecular Dynamics of Blood-Clotting Proteins
• W-Sift, a Structural Interactions Based Potency-Wise Screening Technique for Protein-Small Molecule Complexes
• Microarray Data Mining: A Novel Optimization-Based Iterative Clustering Approach to Uncover Biologically Coherent Structures
• Optimization Based Automated Curation of Metabolic Reconstructions
• In Silico Modification of a Bistable Genetic Network to Obtain Oscillatory Expression Patterns
• Evolution and Changes in the Blosum Matrix and Blocks Database

### Design and Analysis of Green Solvent Systems
***Hilton San Francisco, Continental 5***
• Towards More Sustainable Pharmaceutical Syntheses: Finding Solvent Replacements
• Solvents for Crystallization
• Systems with Ionic Liquids: Measurement and Prediction of Their Thermodynamic Behavior Using Unifac and Cosmo-RS
• Measurement of Distribution Coefficients for Phenols in Ionic Liquid/Water Two-Phase System
• Volumetric Behavior of Water-Alcohol Mixtures at 673.15 K under High Pressures. I. Methanol and Ethanol Solutions
• Computer-Aided Molecular Design for Viscosities and Melting Points of Ionic Liquids
• Vapor-Liquid Equilibria for Methanol + Fatty Acid Methyl Ester Binary Systems near Critical Temperature of Methanol
• Benedict-Webb-Rubin Equation of State for an Alternative Fuel, Dimethyl Ether, and Estimation of Thermophysical Properties

### Developments in Biobased Alternative Fuels
***Hilton San Francisco, Yosemite B***
• Biological Hydrogen Production with Granulation of Hydrogen Producing Bacteria
• Ethanol as Transportation Fuel - Production Technology Developments
• Microbial Conditioning of Corn Stover to Increase Ethanol Yield
• Gaseous Biofuels Production from Sweet Sorghum and Olive Pulp
• Engineering of Cellular Systems for Bioethanol Production Using Global Transcription Machinery Engineering
• Pretreatment of Lignocellulosic Biomass Using Supercritical Fluids
• Pervaporation Membranes Highly Selective for Solvents Produced by Fermentation
• A Novel Lipase Immobilization Technique Using Homopolymer Tethers of Amino Acids
• Fermentation of Acid Pretreated Corn Stover to Ethanol Using Pichia Stipitis
• Kinetic Study of Biodiesel Production from Chinese Tallow Tree Oil
• Directed Evolution of Oxygen-Tolerant Hydrogenase Enzymes for Biological Hydrogen Production
• Fefe Hydrogenases Produced by a Cell-Free Transcription/Translation System

### Devices I
***Hilton San Francisco, Continental 1***
• Exciton Transport in Organic Photovoltaic Cells
• Solving the OLED Outcoupling Problem Using Aperiodic Dielectric Stacks
• Efficient Blue, Green, Orange and White Organic Light-Emitting Diodes Based on an Emissive Oligoquinoline and Different Hole-Transport Materials
• Electrostatic Injection of $10^{15}$ Charges Per Square Centimeter in Organic Semiconductors
• Electrochemical and Electrolyte-Enhanced Polymer Thin Film Transistors

### Drug Delivery (II)
***Hilton San Francisco, Yosemite A***
• The Interplay of Drug, Polymer, and Solvent Properties on the Release Characteristics of Membrane-Based Systems
• Targeting the Breast Cancer Microenvironment Using Interleukin-12 Conjugated Pamam Dendrimers
• Nanoparticles for Targeted Delivery to Prostate Cancer Cells
• Recognition of the Size of Polymer Drug Carriers by Macrophages
• Oral Delivery of Insulin Bioconjugates Using Intelligent Complexation Hydrogels
• Validation of a Model Predicting the Influence of Cyclodextrins on Oral Bioavailability: Comparison with in Vitro and in Vivo Data
• The Characterization of Non-Ionic Surfactant Vesicles: a Release Rate Study for Drug Delivery

### Entrepreneurship and Legal Issues
***Hilton San Francisco, Union Square 21***
• Top Ten Intellectual Property Mistakes Made by Start-up Companies

• Proposed Patent System Survey Curriculum for Undergraduates
• Patent Disclosures: a Resource for Chemical Engineering Education
• Law, Money & Ip
• Entrepreneurship for High School Students and Teachers through Project Lead the Way
• The Case for a Legal Studies Curriculum in Engineering

### Environmental Fate and Transport Processes III
***Hilton San Francisco, Union Square 15 & 16***
• Environmental Management and Sustainability
• Vapor Pressure of Low Volatile Chemicals from a Knudsen Effusion Technique
• Fate and Persistence of Pharmaceuticals and Personal Care Products in Municipal Wastewater
• Steady State Design Model of Concentrations and Fluxes in a Sediment Cap
• Modeling of Ozone Layer Depletion
• Investigation of Heavy Metal Migration in Capping Material and Sediment

### Fuel Cell Membranes II
***Hilton San Francisco, Continental 2***
• Transport in Polymer Electrolytes for Fuel Cells: Physical Chemistry
• Proton Exchange Membranes with Controlled Morphologies
• Development, Structure and Properties of Novel Wholly Aromatic Pore-Filling Electrolyte Membrane for PEMFCs and DMFCs
• Water Transport in a Short Side Chain Psi Membrane: Differences between Cast and Extruded Membranes Subject to Different Thermal Treatments
• Mechanical Properties of Nafion and Nafion/Titania Membranes for PEM Fuel Cells
• Composite Membranes Based on Post-Sulfonated Non-Fluorinated Aromatic Polymers

### Fuel Cells: Fuel Processing II
***Hilton San Francisco, Continental 3***
• Carbon Monoxide Cleanup of Reformate Feed for Proton Exchange Membrane Fuel Cells Using an Electrochemical Membrane Reactor
• Selective Oxidation of Carbon Monoxide to Carbon Dioxide over Cobalt-Based Supported Catalysts for Hydrogen Clean-up in PEM Fuel Cells
• Development of Sulfur Tolerant Reforming Catalyst for Diesel and Jet Fuel: Understanding the Reaction Pathways and Catalyst Characterization
• Cos Formation and Removal Using High Efficient ZnO Based Sorbents for PEMFC Applications

### Genomic Approaches to Systems Biology II
***Hilton San Francisco, Imperial B***
• Automated Pathway Inference from Gene Knockout Data
• Genomic Approaches to Generating Product-Tolerant *Clostridium Acetobutylicum* Strains for Bioprocess Applications
• Systems Analysis of Cellular Response to Alcohol Withdrawal
• Genome-Scale Reconstruction of the Saccharomyces Cerevisiae Signaling Network
• Can We Predict Combined Stress Response from Individual Responses?

### Health and Environmental Effects of Nanoparticles
***Hilton San Francisco, Union Square 14***
• Nanoparticle Occupational Safety and Health Consortium: Aerosol Nanoparticle Behavior and Barrier Efficiency of Filter Media to Engineered Aerosol Nanoparticles
• Managing Uncertainty: a Best Management Practices Approach to Nanoscale Materials and Occupational Health Concerns
• Differential Distribution and Toxicity of Nanomaterials *in Vivo*
• Tools for Aerosol Nanoparticle Exposure Assessment
• Oxide Nanoparticles Uptake in Human Lung Cells
• Use of Physiologically Based *in Vitro* Models of the Gastrointestinal Tract to Study Nanoparticle Absorption and Toxicity
• Stable Colloidal Dispersions of C60 Fullerenes in Water: Evidence for Genotoxicity

### Homogenous and Heterogeneous Atmospheric Chemistry
***Hilton San Francisco, Lombard***
• Mercury Oxidation Via Bromine
• The Chemistry of Mercuric Chloride Reduction in the Flue Gases of Coal Combustion
• Ftir Spectroscopy of Flue Gas Plasma Products
• Pulsed-Corona High Oxidation Reactors in Gas Phase Applications: Effect of the Field Variation on Reactor Conversion
• Receptor Modeling of Surface Aerosols at Beijing (China) and Gosan (Korea) during the Asian Pacific Regional Aerosol Characterization Experiment (Ace) – Asia
• The Oxidation of a Monolayer Organic Surfactant Film on Submicron Aqueous Aerosol
• Isorropia II: a Computationally Efficient Thermodynamic Equilibrium Model for Multiphase Multicomponent Aerosols
• The Influence of Increasing Chemical Complexity on the Hygroscopic Properties of Multi-Component Dicarboxylic Acid Aerosols
• Organic Ccn Activity of *in-Situ* Samples Obtained from the MASE 2005 Campaign
• Probability of the Growth of Ultrafine Atmospheric Aerosol to Cloud Condensation Nuclei

### In Situ and Operando Spectroscopy of Catalysts
***Hilton San Francisco, Franciscan C***
• *in-Situ* Drifts Study on a Model Pt/Ba/$Al_2O_3$ NOx Storage/Reduction Catalyst: the Effect of $CO_2$ and $H_2O$ during Cyclic Operation
• In Situ TEM Characterization of Redox Processes in Ceria-Zirconia
• Smart Combinatorial Operando Spectroscopic Catalytic Reactor System
• Operando Ir/EXAFS Studies of the Promotion Behavior of Pt-$Nb_2O_5$/$Al_2O_3$ Catalysts during the Preferential Oxidation of Co
• No-Assisted $N_2O$ Decomposition with Fe-Ru-Fer: an in Operando XAS and Ir Spectroscopic Study of the Synergy between Fe and Ru
• Supported Rhodium Complexes on Highly Dealuminated Zeolite Y: Characterization during Catalysis of Ethylene Hydrogenation
• Investigation of Solid/Liquid Interfaces by Sum-Frequency Spectroscopy: Acetonitrile Adsorption on Model Supports and Pt Covered Supports

### Life Cycle Analysis of Renewable Feedstock-Based Processes and Products
***Hilton San Francisco, Continental 6***
• Life Cycle Assessment of Integrated Biorefinery: Corn Grain, Corn Stover and Switchgrass
• Considering Advanced Biorefineries in Context
• Life Cycle Analysis of Polyols from Soy Oil or Castor Oil
• Optimal Biorefinery Resource Utilization by Combining Process and Economic Modeling
• Impacts on Soil of Large-Scale Crop Residue Harvest for Biofuel Production
• Techno-Economic Analysis of Lignocellulose to Liquid Fuels Biorefinery Using Aspen Wood as Feedstock
• Life Cycle Assessment of Transportation Fuels Using Hybrid Models

### Microreaction Engineering II
***Hilton San Francisco, Franciscan B***
• Effect of Combustion Mode on Performance and Startup of Microburners
• Thermal Control of Microstructured Reactors through Staged Oxidant Addition
• Remote Controlled Microscale Chemistry
• Novel "Sandwich Microreactor" for Heterogeneous Catalytic Processes:
• Micromixing in Capillary Channels with Buoyancy Flows: Effect of Wall-Based Asymmetric Conditions
• Thermally Integrated Micro-Channel Fuel Processor

### Mixing and Segregation
***Hilton San Francisco, Franciscan D***
• Modeling Radial Mixing and Segregation in Rotating Drums: Effects of Process Parameters
• Axial Mixing of Binary Mixture in Horizontal Rotating Cylinder
• Characterization and Modeling of Continuous Convective Powder Mixing Processes
• Van der Waals Adhesive Forces in Particle Mixing and Segregation
• Segregation of Granular Materials in Couette and Channel Flows
• Electrostatic Crystallization in Shaken Granular Systems
• Understanding the Hydrodynamics and Mixing Behavior in a 2-Dimensional Downer by CFD-DEM Simulation

### Model Reduction, Simulation and Control of Distributed Parameter Systems
***Hilton San Francisco, Van Ness***
• Research of Multi-Dimension Reduction Timing Mutative Scale Constructing Algorithm of Common Basic Data Platform
• Study of Multi-Dimension Reduction Timing Mutative Scale Constructing Algorithm of Common Basic Data Platform
• Control of Particle Size Distribution in an Emulsion Copolymerization Reactor Via Cascade Regulation of Growth and Nucleation
• Optimal Field Reconstruction of Distributed Process Systems from Partial Measurements
• A Dedicated Modal Observer Design for Actuator Fault Isolation in Distributed Control Systems
• Nonlinear Feedback Control of Stochastic PDES
• Modal Model Predictive Control of Kuramoto-Sivashinsky Equation with State and Input Constraints
• Stabilisation of Convection Dominated Problems for the Direct Calculation of Cyclic Steady States of Chemical Processes

### Modeling and Simulation of Fuel Cells and Organic-Semiconductor Systems
***Hilton San Francisco, Union Square 3 & 4***
• First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (SOFC) Anodes
• Ionic Dynamics of Low Temperature Solid Oxide Fuel Cell Electrolytes
• Computational Design of Hybrid Organic/Inorganic Molecular Systems for Electronic Applications
• A Combined Model to Study Conductive Properties of Polymers with Atomic Resolution
• Accurate Prediction of Electron Transport across Organic-Semiconductor Junctions
• Self-Assembly of Organic Semiconductor Molecules: Experiments, Molecular Modeling and Simulation

### Multi-Functional Drug Delivery Systems
***Hilton San Francisco, Sutter***
• Molecular Delivery to Cells Facilitated by Corona Ions
• Enhanced Penetration into Drug-Resistant Tumor Tissue and Cytotoxicity of Doxorubicin Loaded on Gold Nanoparticles
• Polymeric Microneedles Encapsulating Drug for Controlled Release Delivery
• Vaccination Using Topical Formulations
• Encapsulating Indocyanine Green Using Novel Nanoparticle-Assembled Capsules
• Immuno-Targeting of Non Ionic Surfactant Vesicles

• Rigid-Liposomes with Engineered 'Raft-Switches' for Controlled Release of Therapeutics

### Multiphase Mixing II: Solid-Liquid & Liquid-Liquid Mixing

***Hilton San Francisco, California Room***

• Liquid Dissolution: 10 Times Slower Than Blending and 10 Times Faster Than Liquid-Liquid Break-up
• Detailed 3d Evaluation of Oil and Air Dispersion in a Simulated Fermentation Broth, Using a Stereoscopic Vision System
• Modeling Emulsification Using CFD
• CFD Simulations of Low Concentration Particle Distribution in a Viscometer Cup
• Preparation of Highly Concentrated Solid-Liquid Dispersions Using SMX Static Mixers
• Solid-Liquid Two-Phase Flow Simulation in a Maxblend Stirred Tank

### Multiscale Modeling I

***Hilton San Francisco, Union Square 23***

• Probabilistic Molecular Dynamics: Playing Dice with Molecules
• Local Estimation and Coarse-Grained Numerics for Stochastic Reaction Models
• Reduction of Multi-Scale Systems of Chemical Langevin Equations
• Multiscale Modeling of Coupled Drying and Non-ideal Polymerization in Sol-Gel Silica Films
• The Optimal Bidisperse Pore Structure of a Catalyst Chip
• Multiscale Modeling and Analysis: Bridge the Gap between Material Design and Material Application in Surface Coating
• Multiscale Modeling of the Physiological Response of Skin to Focused High Power Microwave Exposure

### Nanoparticle Assemblies and Superlattices

***Marriott San Francisco, Yerba Buena Ballroom 4***

• Inorganic and Organic Nanoparticle Arrays Templated in Thermoreversible Block Copolymer Hydrogels
• Catalytic Activity of Palladium Nanoparticles Encapsulated in Spherical Polyelectrolyte Brushes and Core-Shell-Microgels: Towards "Smart" Carriers Systems
• A Facile Nanoparticle Synthesis/Extraction Strategy to Target Pt Nanoparticle Microarrays and Superlattices
• Assemblies of CdTe Nanowires with Au and Ag Nanoparticles : Exciton-Plasmon Interaction Vs Field-Enhanced Light Absorption
• Modeling Convective Assembly during Colloidal Crystal Growth
• Local Ordering and Stacking Fault Structure in Field-Assisted Assembly of Colloidal Crystals

### Nanoscale Structure in Polymers III: Polymer Nanocomposites

***Hilton San Francisco, Continental 4***

• Calculation of Thermodynamic Stabilities of Polymer/Carbon Nanotube Composites
• Average and Local Distribution of Glass Transition Temperatures of PMMA-SWCNT Nanocomposites Studied Via Fluorescence
• Mechanical Properties of SWNT-Polymer Composite Thin Films Fabricated by Molecular Layer-by-Layer Assembly Technique
• Mechanisms of Steady-Shear Rheology in Polymer-Nanoparticle Composites
• Polymer-Graphite Nanosheet Composites Via Solid-State Shear Pulverization: a Robust and Practical Approach to Effective Nanofiller Dispersion
• Nanocomposite Fabrication through Particle Surface Initiated Polymerization
• Structure and Rheology of Supercritical Carbon Dioxide-Based Dispersed Polymer Nanocomposites

### Novel Electrochemistry and Materials for Fuel Cells I

***Hilton San Francisco, Continental 7***

• Development of Iron-Based Perovskite Materials as Carbon and Sulfur Tolerant Solid Oxide Fuel Cell Anodes
• Defect Structure for Proton Transport in a Triflic Acid Monohydrate Solid
• Development of Compression Moldable Polymer Composite Bipolar Plates for Fuel Cells
• Novel Non Noble Metal Catalysts for Oxygen Reduction Reaction
• Oxygen Electroreduction on Au-Co Bimetallic Nanoclusters in Alkaline Solutions
• Pt-Ru Nanoparticles Supported on Carbon Nanotubes as Methanol Fuel Cell Catalysts
• Performance of a First-Generation Biocarbon Fuel Cell

### Novel Membranes and Membrane Processes for Water Treatment and Production

***Hilton San Francisco, Plaza B***

• Modeling of Direct Contact Membrane Distillation of Saline Water in Cross Flow Hollow Fiber Devices
• Technical and Economic Feasibility of Reverse Osmosis Reclamation of Agricultural Drainage Water in the San Joaquin Valley
• Internal Concentration Polarization in Forward Osmosis: Influence of Membrane Orientation and Operating Conditions on Flux Performance
• Membrane Bioreactor Process Model for the Removal of Biodegradable Organic Matter and Disinfection Byproduct Precursors from Water Supplies
• Electrodialysis/Reverse Osmosis to Recover Dissolved Organics from Seawater
• Membrane Fouling and Transport Models in Water Treatment Applications

### Plasma Processing I - Co-Sponsored by the American Vacuum Society

***Marriott San Francisco, Yerba Buena Ballroom 5***

• Effect of the Number of Layers of Dielectric Barrier Discharge Reactor on Diesel Particulate Matter Removal and Pressure Drop
• Inertial Gas Admixtures in Pecvd for Uv Absorbing Thin Films of Titanium Dioxide on Polymers
• Plasma Treatment of Low Density Polyethylene (LDPE) Using an Low-Temperature Cascade Arc Torch
• Diagnostics of Inductive-Coupled Ch2f2/CF4 Plasma Using Langmuir Probe and Quadruple Mass Spectrometry
• Ion-Enhanced Plasma Etching of Hafnium Aluminates in Chlorine Based Plasmas
• Plasma Interface Engineered Coating Systems for Magnesium Alloys
• Surface Reactions in Plasma Etching of Nitrided Hafnium Silicates

### Polymerization Reaction Engineering, Kinetics and Catalysis II

***Marriott San Francisco, Yerba Buena Ballroom 6***

• Enzyme-Catalyzed Miniemulsion Polymerization
• Silica Tethered Sulfonic Acids for Activation of Olefin Polymerization Catalysts
• Syndiotactic Styrene Polymerization on a Flat-Surface Deposited Metallocene Catalyst
• The Early-Time Polymerization Kinetics in Acidic Water/Alcohol Solutions of Bis(Trialkoxysilyl) Alkanes with Short Bridging Chains
• Inhibitive Chain Transfer to Ligand in Atom Transfer Radical Polymerization of *n*-Butyl Acrylate
• Kinetic Study of the Solution Polymerization of Methacrylamide Initiated with Potassium Persulfate Using *in-Situ* Raman Spectroscopy and Novel Multivariate Data Analysis – Band-Target Entropy Minimization (BTEM)
• Application of on-Line Ft-NIR Spectroscopy for Monitoring the Kinetics of Anionic Polymerizations

### Protein Product Drug Formulation and Delivery

***Hilton San Francisco, Powell***

• A Study on Release of Therapeutic Proteins from L-Tyrosine Based Novel Polyphosphate Microparticles
• Sustained Drug Delivery of an Integrin Antagonist for Ocular Angiogenesis
• Amine-Functionalized SBA-15 on Protein Delivery: Adsorption, Release and Stability of Bovine Serum Albumin
• Nanoporous Drug Delivery Devices Based on Functional Polymers
• Sub-Micron Scale Dispersion of Protein in a Polymer Matrix
• A Method for Three Dimensional Protein Characterization and Its Application to a Complex Plant (Maize) Extract
• Simultaneous Phase Transition of Elp Tagged Molecules and Free Elp: a Specific, Efficient and Reversible Molecular Recognition System

### Scheduling

***Hilton San Francisco, Union Square 5 & 6***

• Smart Plant I
• Smart Plant II
• Optimal Scheduling of Multistage Batch Plants with Sequence Dependent Changeovers: a Comparative Study
• An Improved Continuous-Time Model for Short-Term Scheduling of Continuous Processes: Rigorous Treatment of Storage Requirements
• Optimal Integration of Production Planning and Process Operation in Petrochemical Industry
• A Continuous Approach to Multi-Mode Resource Project Scheduling
• Task Selection, Assignment and Sequencing in Multistage Batch Processes
• An Efficient Routine to Increase Robustness of Production Plans Embedded in an Integrated Multi-Scale Planning and Scheduling Approach

### Separation of Processing Streams Derived from Renewable Feedstocks

***Hilton San Francisco, Continental 9***

• Biosep: a New Ethanol Recovery Technology for Small Scale Rural Production of Ethanol from Biomass
• Concentration of Proteins from Switchgrass and Distiller's Grains Using Ultrafiltration during Biomass Refining
• Nanofiltration & Separation of Hydrolyzates from Sugar Maple Wood
• Cost Effective High Value-Added Chemical Extraction from Lignin with Gas Expanded Liquids
• Fractionation of Hot-Water Wood Extracts
• Solids Handling for Biorefinery Integration Using Process Engineering Simulators

### Tissue Engineering: Stem Cells in Tissue Engineering (II)

***Hilton San Francisco, Yosemite C***

• Effect of Immobilized Glycosaminoglycans on the Expansion of Megakaryocyte Precursors and Cd34+ Cord Blood Stem Cells
• Quantitative Modeling of Metabolically Mature Na-Butyrate Induced Hepatocyte-like Cells from Embryonic Stem Cells
• Stem Cell Microarrays: Investigation of Factors That Influence Neural Stem Cell Fate
• Culture under Reduced Oxygen Dramatically Increases Differentiation of Murine Embryonic Stem Cells into Cardiomyocytes
• Differentiation and Apoptosis in Megakaryocyte-Directed Hematopoietic Stem Cell Cultures
• Vitronectin and Collagen I Differentially Regulate Osteogenesis in Mesenchymal Stem Cells
• Effects of Shear Stress on 3-D Human Mesenchymal Stem Cell Construct Development under Perfusion

**Transport Phenomena in Electronic Materials Processing**
***Marriott San Francisco, Yerba Buena Ballroom 2***
• Multi-Scale Simulation of Quantum Dot Formation in Metal Thin-Film Epitaxy
• Multiscale Modeling and Neural-Network Based Optimization of a Thin Film Deposition Process
• Analysis of Electromigration-Driven Interactions between Voids in Metallic Thin Films
• Effect of Rotational Speed and Marangoni Stresses on Local Flow Structure in Silicon Melt of Czochralski Crystal Growth Process
• Defect Engineering by Short-Annealing-Time Methods for Ultrashallow Junction Formation
• A Comprehensive Model for Coupled Oxide Precipitation and Point Defect Aggregation in Crystalline Silicon

**Transport Phenomena in Fluid-Particle Systems**
***Hilton San Francisco, Continental 8***
• Plasma Treatment of Diamond Nanoparticles for Dispersibility Improvement
• Computational Particle-Fluid Dynamics Simulations of a Commercial-Scale Turbulent Fluidized Bed Reactor
• A Computational Framework for Studying Particle in-Flight Behavior in the HVOF Thermal Spray Process
• Investigating Wide Shear Zones in Slow Granular Flow by Discrete Element Simulations
• Experimental Investigation and CFD Modeling of Liquid-Solid Flow with Particle-Particle Collisions
• Direct Simulations of Inertial Effects on Flexible Cylindrical Fiber in Flows

**Water Treatment and Characterization - Novel Methods and Non-Traditional Water Sources**
***Hilton San Francisco, Grand Ballroom A***
• Integration of DCMD Modules in a Cascade for Energy Efficient Desalination/Purification
• Removal of Methyl Tert-Butyl Ether (MTBE) from Water by Membrane Air Stripping
• Principals of Managed Irrigation with Coal Bed Natural Gas Produced Water
• Development of Filtration/ Biotreatment Scheme to Recycle CMP Wastewater
• Drinking Water Corrosion Control Treatment - Small Systems Case Studies
• Limitations and Solutions for Biological Reactors in Microgravity Compatible Water Reuse Systems

**FRIDAY, 17 NOVEMBER 2006**
***8:30 AM - 11:00 AM***
**Advances in Co Hydrogenation I**
***Hilton San Francisco, Franciscan C***
• Effects of Support Composition on the Activity of Cu/MxZr1-$XO_2$ (M = Ce, Pr, Mn) for Methanol Synthesis Via Co Hydrogenation
• The Effect of Rhodium Precursor on Carbon Monoxide Hydrogenation Catalysts
• Fischer-Tropsch Synthesis: Characterization of Interactions between Reduction Promoters and Co for Co/$Al_2O_3$–Based GTL Catalysts
• An Investigation into Supercritical Fluids as a Reaction Media for Fischer Tropsch Synthesis
• Synthesis, Activation, and Mechanism of Function for Fischer-Tropsch Synthesis Catalysts Based on Iron
• Fischer-Tropsch Synthesis: Comparison of $^{14}C$ Distributions and Analysis of Reaction Pathways When Labeled Acetic Acid Is Added
• Development of a New Kinetic Expression for the Iron-Based Fischer-Tropsch Reaction

**Advances in Computational Methods and Numerical Analysis I**
***Hilton San Francisco, Continental 2***
• Numerical Analysis of the Nonlinear Deformation and Breakup of Semi-Insulating Electrified Liquid Jets
• Multiscale Discontinuous Galerkin Methods for Simulating Single-Phase and Multi-Phase Flow in Porous Media
• Theoretical Development and Industrial Application of a Geometrically-Based Criterion for Film Uniformity Control in a Planetary Sic CVD Reactor System
• Design and Validation of a Numerical Problem Solving Environment for Ordinary Differential Equations
• Faster Methods for Solving Large Quadratic Programs
• Role of Sampling in Process Design, Optimization and Control

**Advances in Electrokinetics and Electrophoresis - Fundamentals**
***Hilton San Francisco, Grand Ballroom A***
• Application of Charged Membranes in Electroosmotic Pumping
• Investigating the Link between Changes in Surface Characteristics and Protein Expression for Aggregated and Non-Aggregated Bacillus Cereus
• Performance Bottlenecks in Dynamic Field Gradient Focusing
• Quantitative Analysis of the Binding of Monovalent Cations by Oligonucleotides
• Optimal Separation Times in an Electrokinetic Couette-Based Device: an Area-Averaging Approach with Orthogonal Fields
• Electrokinetic Transport of Charged Analytes through Nanofluidic Channels

**Advances in Environmental Technology: Green Bioprocessing**
***Hilton San Francisco, Yosemite B***
• Biotransformation of Olive Mill Wastewater into Valuable Products through Biohydrogen Processes
• Commercial Production of Polyhydroxyalkanoates in Tomato Cannery Wastewater Treatment
• Production of Galacto-Oligosaccharides from Whey Lactose by Immobilized Enzyme ß-Galactosidase from *Aspergillus Oryzae* and *Bacillus Circulans* with Chromatographic Separation
• Recombinant Expression, Stability and Purification of the Lignin Oxidizing Enzyme Manganese Peroxidase
• Evolution in Reverse: Engineering a Xylose-Specific Xylose Reductase
• Ethanol Production from the Fermentation of Synthesis-Gas
• The Biorefinery Concept in Brazil

**Advances in Extreme Biocatalysis**
***Hilton San Francisco, Yosemite A***
• Bioconversion of Biomass Using a Co-culture of *Thermotoga Maritima* and *Methanococcus Jannaschii*
• Thermoacidophilic Cellulases and Hemicellulases from Alicyclobacillus Acidocaldarius
• Complex Hyperthermophilic Proteases: the Effect of Beta Protein Content on Biochemical and Biophysical Properties of Proteasomes
• Effects of Mass-Transfer and Kinetic Parameters on Biocatalytic Activity of Immobilized Burkholderia Cepacia Lipase in a Packed-Bed Reactor
• Regulation of Carbon Monoxide Dehydrogenase Gene Complexes by Cooa in *Carboxydothermus Hydrogenoformans*
• Proteomic Analysis of a Hydrogen Producing Thermophile *Carboxydothermus Hydrogenoformans*

**Alternative Fuels and Enabling Technologies III**
***Hilton San Francisco, Continental 9***
• Reduction of Metal Oxide Particles with Syngas for Hydrogen Production
• Enhancement of Dimethylether Yield by Reverse Shift Reaction in the Direct Dimethylether Synthesis
• Biogas Production Using Glycerol, the Biodiesel by-Product, as the Carbon Source
• Synergism between Coal Gasification and Ethanol Production
• Stability Assessment of Wood and Bark Derived Bio-Fuels
• High Purity Hydrogen Production with *in-Situ* Carbon Dioxide and Sulfur Capture

**Applied Mathematics in Bioengineering I**
***Hilton San Francisco, Continental 4***
• Stochastic Modeling and Monte Carlo Simulation of the Temporal Evolution of Phenotypes *R5*, *R5X4*, and *X4* of Human Immunodeficiency Virus Type 1
• An Adaptive Time Stepping Scheme for Systems of Stochastic Differential Equations with Multiple Multiplicative Noise. Chemical Langevin Equations, a Proof of Concept
• Quantifying the Effect of Cell Population Heterogeneity on Proliferation Rates
• Quantitative Assessment of Biofitness in Heterogeneous Bacterial Populations under Antibiotic Pressure
• Solution Multiplicity of Inversion Problems in Distributed Systems
• Stochastic Population Balance Modeling of Influenza Virus Replication in a Vaccine Production Process
• A Mathematical Model for Citric Acid Fermentation by Aspergillus Niger
• Fluorescence Microscopy –Based Inverse Cell Population Balance Modeling

**Biological Conversions and Processes for Renewable Feedstocks II**
***Hilton San Francisco, Continental 7***
• Expression of Novel Enzymes for Biomass Conversion in *E.Coli*
• Enzymatic Processing of Corn Fibers for a Complete Recovery of Ferulic Acid and Fermentable Sugars
• High-Value Lignin Co-Products through Pretreatment and Microbial Conditioning
• Genomics Enabled Optimization of E. Coli Succinate Production
• Conversion of Glucose, Xylose, and Glycerol by *Rhodotorula Glutinis* into Triglycerides a Biodiesel Feedstock
• Biorefining Mixed Sugars Using High Densities of Growth-Arrested Corynebacteria
• Development of Cereal-Based Biorefineries for the Production of Biodegradable Plastics and Platform Chemicals

**Biosensors I: Cancer and Biotoxin Detection**
***Hilton San Francisco, Sutter***
• A Novel Biosensor System on Microfluidic Platform for Diagnosis of Breast Cancer
• Colon Cancer Marker Detection in Human Serum Using a Surface Plasmon Resonance Sensor
• Development of Rapid Nano-Structured Sensor System for Category BToxins Detection in Complex Biological and Environmental Samples
• Ultrasensitive DNA Sequence Detection Using Nanoscale Zinc Oxide Sensor Arrays
• Impedimetric Immunosensor for Ricin Detection in Low pH Foods
• Detection of Organophosphorus Compounds Using an Acetylcholinesterase-Based Biosensor
• Development of Spr Sensor Receptor Binding Assay to Detect Paralytic Shellfish Poisoning Toxins

**Biotechnology Tutorial & Panel Discussion**
***Hilton San Francisco, Imperial B***
• Bioreactor Technology
• Mixing Issues in Large Scale Stirred Bioreactors: Animal Cell Culture as an Example
• Centrifugation as a Method of Primary Recovery for Cell Culture Products
• Trends and New Developments in Filtration
• Chromatography for Downstream Processing of Therapeutic Proteins – Current Status and Future Challenges
• Tutorial Panel Discussion

**Cape-Open Numerical Components: Development and Usage**
***Hilton San Francisco, Union Square 5 & 6***
• Review of Cape-Open Numerical Interfaces

Implementations
• Fast Co-Simulation of Advanced Power Plants Using Neural Network Component Models
• Cape-Open Compliant Multi-Objective Optimization Capability for Apecs Systems
• Cape-Open Compliant Stochastic Modeling and Reduced-Order Model Computation Capability for Apecs System
• An Integrated Simulation-Optimization Framework for Waste Minimization Analysis in Chemical Plant
• Dynamic Cape-Open Simulation Approach on Cluster Oriented Architecture
• Panel Discussion

**Computational Biology: Systems Modeling II**
***Hilton San Francisco, Union Square 17 & 18***
• Characterizing the Interval Timer within *Drosophila*'s Circadian Clock
• Analyzing Individual Cancer Cell Motility with Chemotaxis Perspective
• A Combined Modeling and Experimental Approach for in Vivo Parameter Estimation
• Characterization of Cross-Hybridization Via Stochastic Simulation
• Improved Logical Formulation for Transcription Regulatory Networks Reconstruction Via Integer Linear Programming
• Deterministic and Stochastic Modeling of Genetic Networks with Positive Feedback Architecture
• Modeling Ire1p Regulation and Activation in the Yeast Upr
• Adhesive Dynamics Simulations of the Shear Threshold Effect for Leukocytes
• Molecular Mechanisms of HIV-1 Latency: Stochastics in Gene Expression and Chromatin Regulation

**Computational Catalysis I**
***Hilton San Francisco, Franciscan A***
• Nitrous Oxide Decomposition over Fe-ZSM-5 in the Presence of Nitric Oxide: a Comprehensive DFT Study
• A Theoretical Comparative Study of Fischer-Tropsch Synthesis on Fe and Co Surfaces
• Heterogeneous Catalysis by Gold: Oxide-Specific O2 Interactions with Supported Gold
• A DFT Study of Olefin Polymerization by Ti and Zr Single-Site Catalysts Containing Mixed Cyclopentadienyl/Aryloxide Ligation
• Correlating Electronic Properties of Bimetallic Surfaces with Reaction Pathways of C2 Hydrocarbons
• Ab Initio Studies of Oxygen Electroreduction on Pd and Pd/3d Metal Alloys

**Design, Analysis and Operations under Uncertainty I**
***Hilton San Francisco, Continental 1***
• Steady-State Optimization with Guaranteed Stability under Parametric Uncertainties
• Hedging Risk through the Flexible Recipe Framework
• Design of Uncertain Discrete Time Systems with Constructive Nonlinear Dynamics Methods
• Scheduling under Uncertainty Using Parametric Programming
• Quantifying Risk in Multistage Stochastic Problems Using Approximate Dynamic Programming and Coherent Risk Measures
• Propagation of Uncertainties in Nonlinear Dynamic Models
• Analysis and Evaluation of Batch Chemical Processes under Uncertainty Using Process Simulation and Risk Analysis Tools
• Dynamic Programming for Uncertain Multiparametric Problems

**Devices II**
***Hilton San Francisco, Union Square 3 & 4***
• Stability of Polymeric Thin-Film Transistors
• Inkjetted Organic Transistors for Smart Tagging Applications
• Printed Organic Field Effect Transistor with Solution Processed Nanocomposite Dielectric Gate Insulator
• Dielectric Materials for Low Operating Voltage Organic Thin-Film Transistors
• High-Performance, Microscale Field-Effect Transistors for the Probing of Charge Transport in Molecular Crystals

**Fuel Cell and Microchemical Systems Modeling**
***Hilton San Francisco, Taylor***
• Multi-Scale Modeling and Control of Autothermal Reactors for the Production of Hydrogen
• Design of Portable Power Generation Systems for Variable Power Demand
• A Novel AC Impedance Model for Electrochemical Devices
• Optimization Study of Proton Exchange Membrane Fuel Cells (PEMFC) for Platinum Reduction and Performance
• Validation of a Phenomenonological Steady-State Model for Solid Oxide Fuel Cell (SOFC)
• Control–Relevant Design of Electrochemical Hybrid Power Systems Using Dynamic Optimization Methods
• The Impact of Hydration Dynamics on the Control of a PEM Fuel Cell

**Green Materials: Forest and Biobased Products I**
***Hilton San Francisco, Union Square 22***
• Ecobionanocomposites: a New Class of Green Materials from Poly(Lactic Acid) and Cellulosic Nanowhiskers
• Biodegradable Nanocomposites from Wheat Straw
• Bio-Nanocomposites Based on Cellulose Whiskers
• Nanoporous Carbon from Corn Cobs for Methane Storage
• Comparison of Soxhlet Extraction and Back-Flush Filtration for Removal of Homopolymer from Starch-G-PMMA Synthesized with and without Photoinitiator

**Industrial Innovation in Process Design & Operations**
***Hilton San Francisco, California Room***
• Integration of Product Development, Process Design, and Operation on a Kilo-Plant
• Optimal Operating Policies for Process Chemistries with Multiple Chemical Reactions
• Short-Term, Medium-Term, and Reactive Scheduling of an Industrial Polymer Batch Plant
• Scale-up and Control of Fluidized Bed Production of Solar-Grade Silicon
• Integration of Cyclic Hoist Scheduling and Water-Reuse Network Design for Environmentally Benign Manufacturing
• Multi-Objective Design Optimization of an Industrial LDPE Tubular Reactor Using Jumping Gene Adaptations of Nsga and Constraint Handling Principle
• Temporal Mixing for Attenuation of Time Dependent Variations

**Mixing Issues in Industrial Processes II**
***Hilton San Francisco, Union Square 23***
• 2006 NAMF Award Winner Presentation — Fluid Mixing in the Pharmaceutical Industry: Challenges and Opportunities
• Finding the Right MIX of Computational Fluid Dynamics and Industrial Fluid Mixing Practice in the Design and Analysis of Stirred Tank Reactors
• Pilot-Scale Studies of Requirements for Suspending Settled Solids in SRS Process Tanks
• How to Specify (or Not Specify) Mixers for Solids Suspension
• KT-3: a Novel Tickler for Solids Removal from Slurry Vessels
• Experimental Techniques for Contacting of Solids with Heavy Hydrocarbon Liquids for High Temperature Conversion in Co-Rotating Twin Screw Mixers

**Multifunctional Reactors**
***Hilton San Francisco, Franciscan B***
• Application of Equilibrium Theory for Analysis of Non-Isothermal Chromatographic Separations and Chromatographic Reactors
• Process Development for the Synthesis of Dimethylacetal in Simulated Moving Bed Reactor
• A Novel Concept in Adsorption-Enhanced Hydrogen Production
• Study of Ru/Sic Monoliths for the Production of Hydrogen: Ammonia Decomposition and Propane Steam Reforming
• Steady State and Dynamic Studies of NOx Storage and Reduction with Hydrogen and Carbon Monoxide on Pt/Ba/Alumina Monoliths

**Multiscale Modeling II**
***Hilton San Francisco, Union Square 15 & 16***
• Multiscale Simulations of Ortho-Terphenyl in Bulk and Freestanding Films
• Determination of the Onset of Structural Transitions in Condensed Matter through Coarse Molecular Dynamics
• The Properties of Asymmetric Binary Lennard-Jones Mixtures Using Coarse-Grained Two-Body Effective Potentials
• Coarse-Grained Lattice Kinetic Monte Carlo Simulations of Defect Aggregation in Crystalline Silicon
• Mesoscale Simulations of Hydrated Nafion Membranes
• Calculation of Local Pressure Tensors in Systems with Many-Body Interactions
• Multiscale Simulation of Self-Assembly of Nanoparticles in Diblock Copolymers
• Integrated Process and Product Analysis for Automotive Paint Spray: a Multiscale Approach

**Nano-Biotechnology: Development, Application, and Societal Impacts on Sustainability**
***Hilton San Francisco, Continental 5***
• Development of a Biofuel Cell Using Redox-Polymer-Grafted Carbon Electrode
• Site-Specific Protein Manipulation Utilizing Transglutaminase and Its Potential in Nano-Biotechnology
• Intramolecular Electron Transfer in a Novel Cytochrome P450cam System with a Site-Specific Branched Structure
• The Effect of Patterned Silicone Surfaces on Bacterial Adhesion
• Peptide Engineering for Bio-Inspired Zinc Oxide Materials
• Enzyme Immobilization in Mesoporous Carbons for Bioelectrochemical Applications

**Nanoelectronic Materials**
***Hilton San Francisco, Plaza B***
• Directed Bottom-up Self-Assembly into Top-down Features Defined for Precise Positioning of Individual Silicon and Germanium Nanoparticles on Amorphous Substrates
• Systems Tasks in Nanotechnology Via Hierarchical Multiscale Modeling: Self-Assembled Nanopattern Formation in Heteroepitaxy
• Relaxation of Biaxial Strain in Ultra-Thin Films of Face-Centered-Cubic Metals: Ductile Void Growth and Nanocrystalline Domain Formation
• Optoelectronic Polymer Nanowires Via Temple Wetting
• Non-Catalytic and Template-Free Growth and Photoluminescence of Aligned CdS and Cd1-XZnxS Nanowires
• Biological Fabrication of Metal Oxide Nanostructures Possessing Novel Optoelectronic Properties
• Atomic-Scale Analysis of Structural and Mechanical Properties of Microporous and Mesoporous Amorphous Silicas

**Novel Electrochemistry and Materials for Fuel Cells II**
***Hilton San Francisco, Continental 8***
• Accelerated Membrane Chemical Degradation and Diagnostic Methods
• Stability of Platinum-Based Alloy Cathode Cata-

lysts in PEM Fuel Cells
• The Effects of Cationic Contamination on PEM Hydrogen Fuel Cells
• Porous Crystalline Organosilica Materials as High Surface Area Support in Proton Exchange Membranes for Fuel Cells
• Synthesis and Characterization of Microporous Titanium Silicates for Use as Proton Conducting Materials

**Plenary: Frontiers in Energy Usage and Policy**
***Hilton San Francisco, Continental 6***

**Polymer Thin Films and Interfaces IV**
***Hilton San Francisco, Union Square 25***
• Surface-Initiated Ionomer Films Based on Modified Poly(Norbornene)
• Initiated Chemical Vapor Deposition of Polymer Thin Films
• Multipotent Polymer Coatings Based on Chemical Vapor Deposition Copolymerization
• Ultrasonic Non-Destructive Evaluation of Adhesive Thin Layer
• Density Functional Approach for Modeling Polymer-C02 Interfaces
• Chemical Vapor Deposition within Confined Microgeometries
• Welding Immiscible Polymer with $CO_2$
• The Role of Gibbs Excess Adsorption on Submerged Surfaces in Explaining the Complex Swelling Behavior of Supported Polymeric Thin Films in Supercritical Carbon Dioxide
• Nanoscopic Wrinkled Morphology of Polyelectrolyte Multilayer Films on Poly(Dimethylsiloxane) Substrates Induced by Thermal Crosslinking

**Process Development Tools for Pharmaceutical Process Development**
***Hilton San Francisco, Franciscan D***
• Shear-Induced Compaction of Pharmaceutical Formulations
• A Numerical Investigation of Air Flow during Tablet Compression
• Combined Experimental and Modeling Study of a Kinetic Resolution
• On-Line Ftir Measurements for the Pilot-Plant Scale-up of a Borane Reduction Process
• Development of a Generic Process Model for Dynamic Simulation of Protein Downstream Processes
• Catalyst Trap Microreactor for Pharmaceutical Hydrogenation
• Ion Exchange Process Development with Pat

**Process Modeling and Identification I**
***Hilton San Francisco, Union Square 14***
• An Input/Output Approach to Control of Distributed Chemical Reactors
• Estimation of Noise Covariances and Disturbance Structure from Data Using Least Squares with Optimal Weighting
• Gray-Box Modeling of an Integrated Plant with Incomplete Dynamic Information
• Practical Challenges in Bayesian Modeling and Elicitation of Probabilistic Information
• An Optimization-Based Approach to Improving the Identifiability of Nonlinear Large-Scale Systems
• A Continuous-Discrete Extended Kalman Filter Algorithm for Prediction-Error-Modeling
• Accurate Model Identification for Non-Invertible Mimo Sandwich Block-Oriented Processes

**Properties and Design of Biobased Products**
***Hilton San Francisco, Union Square 21***
• High-Performance Nanofibers and Nanostructures for New Generation Multifunctional Materials
• Thermal Conductivity of Coated Paper
• Magnesium Hydroxide Nanoparticle Based Flocculation and Retention System
• Diffusivity Calculations in Paper Materials
• Fiber Dissolution Using NaOH/Urea Solution

**Reactor Engineering for Biomass Feedstocks**
***Hilton San Francisco, Continental 3***
• Mixing and Scale-up of Stirred Tank Reactors Using CFD Simulations
• Production of Sugars from Cellulose in Subcritical and Supercritical Water Using a Non-Isothermal Reactor
• Hydrothermolysis of Agricultural Waste
• Production of Biochemicals from Rice Husk Using a Membrane Reactor under Hydrothermal Condition
• Reactor Development for Partial-Oxidative and Catalytic Gasification of Biomass in Supercritical Water
• Ammonia Formation Rates in Biomass Pyrolysis
• Optimization of Flash Carbonization(Tm) Conditions for Charcoal Production from Sunflower Shells

**Receptor Mediated Phenomena**
***Hilton San Francisco, Yosemite C***
• Integrated Models of Leukocyte Signaling and Adhesion
• Manganese and Gadolinum Regulate Neutrophil Cd18 Integrin Affinity Via Distinct Mechanisms
• Elucidating the Sequential Binding of Lfa-1 and Mac-1 to Icam-1 under Shear Conditions: Possible Role of E-Selectin Signaling
• Spontaneous Activation of Pi 3-Kinase Signaling during Fibroblast Spreading Is Affected by Surface Rigidity and Cytoskeletal Signaling Components
• Experimental and Computational Analysis of Notch1 Receptor Signaling in Adult Neural Stem Cell Differentiation
• Autologous Chemotaxis of Tumor Cells: a Novel Homing Mechanism to Lymphatics
• Autocatalytic Activation of a Viral Fusion Protein

**Semiconductor Surface Chemistry**
***Hilton San Francisco, Powell***
• Impact of Surface Chemistry and Mg:O Flux on Magnesium Oxide Thin Film Heteroepitaxy on Hexagonal Silicon Carbide for Integration of Functional Oxides
• Probing Interactions of Ge with Chemical and Thermal $SiB0_2$ to Understand Selective Growth of Ge on SiB during Molecular Beam Epitaxy
• Investigations of Silane Adsorption and Reaction on Oxygen-Covered Metal Surfaces
• Surface Chemistry for the Growth of Epitaxial Oxide Layers on SiB(001)-2x1
• STM Manipulation and First Principles Simulation of a Molybdenum Disulfide Surface
• Surface Chemistry of Ferroelectric Lithium Niobate
• The Role of Dative Bonding in the Reactivity of Semiconductor and Metal Oxide Surfaces

**Supramolecular Assembly of Inorganic Materials II**
***Hilton San Francisco, Plaza A***
• Block Copolypeptides: Biomimetic Soft Matter and Its Use to Assemble Hard Matter
• Carbamate-Dendrimer Directed Synthesis and Characterization of Uniform-Size Shell Cross-Linked Nanocages with Hydrophobic Interior Walls and Functionalized Cores
• Controlling Interfacial Curvature of Self-Assembled Mesoporous Thin Films by Controlling Cluster Size
• Organizing Inorganic Nanoparticles into Microcapsules Using Polymer Aggregates
• Mechanistic Links between Mesoporous and Microporous Silicate Synthesis
• Fabrication of Distorted Cubic Mesoporous Silica Film Employing a Hydrophobic Organic Additive
• Hierarchical Silica Particles by Dynamic Multicomponent Assembly

**Sustainable Engineering in Process Development**
***Hilton San Francisco, Union Square 1 & 2***
• Economical Comparison of Different Technologies for Biodiesel Production
• Development of a New Energy Concept for an Aluminium Processing Company
• Critical Challenges in Developing Solar Thermochemical Water Splitting Cycles for Renewable Hydrogen
• Robust and Flexible Framework for Optimization of Biorefinery Production
• A Superstructure Optimization Approach for the Design of Corn-Based Ethanol Plants
• Chemical Looping Reforming – an Efficient Process for the Production of Hydrogen from Coal
• Carbon Dioxide in Chemical Processes

**The Third Industrial Fluid Properties Simulation Challenge**
***Hilton San Francisco, Union Square 19 & 20***
• Talks for this session will be chosen from the winners of the IFPSC competition.

**Topics in Surface Science and Catalysis I, In Honor of Robert J. Madix**
***Hilton San Francisco, Imperial A***
• Formic Acid on Transition Metals: from Fundamental Measurements to Practical Devices
• All That Glitters Is Not Gold – Lessons from Surface Science and Catalysis on Silver
• Removal of Alkanethiols from a Hydrocarbon Mixture by Heterogeneous Reaction with Metal Oxides
• Elucidating Carbonyl Chemistry on Ge(100)-2x1
• Surface Functionalization of Aerosolized Silicon Nanoparticles
• Selective Addition of O and Nhpromoted by Au
• Ethanol Conversion on Pt and Pt-Sn Alloys: Surface Reactions and Intermediates

**FRIDAY, 17 NOVEMBER 2006**
***12:30 PM - 3:00 PM***
**(22c) Nanowires III: Integration of Nanowires**
***Hilton San Francisco, Plaza B***
• Nanowire Self-Assembly Using Surface Forces
• Germanium Nanocrystals and Nanowires: Morphological Control, Surface Characterization, and Applications
• Magnetically Assembled and Magneto-Transport Studies of Single Ferromagnetic Nanowires
• Creating Polymer-Templated Nanowire Array
• Selective Growth of Zinc Oxide Nanowires from the Edge of Thin Film Multilayer Structure for Shadow Lithography
• Device Integration of the ETS-4 Quantum Wire Arrays

**Advances in CO Hydrogenation II**
***Hilton San Francisco, Franciscan C***
• Fischer-Tropsch Synthesis: a Comparison of Iron and Cobalt Catalysts
• Adsorption/Reaction of Co on Fe Fischer-Tropsch Catalysts
• Carbon Nanotubes as a Support for Fischer-Tropsch Catalysts
• Effect of Potassium on Oxygenates and Hydrocarbons over Carbon-Supported Iron Catalysts
• Spray Dried Iron Catalysts for Slurry Phase Fischer-Tropsch Synthesis
• Slurry Phase Fischer-Tropsch Synthesis Catalyzed by Nano-Sized Iron: Effect of Particle Size
• Modifications of Fischer-Tropsch Product Distribution in Modular Reactor Systems

**Advances in Computational Methods and Numerical Analysis II**
***Hilton San Francisco, Continental 2***
• A Universal Approach for Error Characterization for Monte Carlo and Quasi Monte Carlo Sampling

• A Bayesian Approach to Mathematical Model Building
• Computational Methods of a Generic Motif Discovery Algorithm for Sequential Data
• Projective and Coarse Projective Integration for Multiscale Problems with Continuous Symmetries
• A Family of Esdirk Solvers for Dae Systems
• Numerical Algorithms for Solving Population Balance Equations Using Quadrature Based Moment Methods

### Advances in Nonlinear Control
***Hilton San Francisco, Union Square 13***
• A Fast and Efficient Computational Framework for Large-Scale Nonlinear Model Predictive Control
• Integrating Feedback and Supervisory Control of Hybrid Nonlinear Processes with Uncertain Mode Transitions
• Fault-Tolerant Output Feedback Control of Multivariable Nonlinear Processes
• Decentralized Multi-Agent Control of Distributed Reactor Networks
• Robust Model Predictive Control of Nonlinear Processes with State, Input and Rate Constraints
• On the Role of Directionality in Analytical Model Predictive Control
• Multi-Component Batch Distillation Control

### Alternative Fuels and Enabling Technologies IV
***Hilton San Francisco, Continental 9***
• Detailed Energy Assessment at Oil Refinery: Tools and Results
• Chemical Recuperation of Low-Grade Exhaust Heat by Steam Reforming of Dimethyl Ether
• Crude Unit Expansion Study for Attock Refinery Ltd
• Modeling and Simulation of Biomass Pyrolysis as a First Step in a Gasification-Based System
• Measurements of the Calorific Value of Volatiles and Oxygen Demand of Solid Fuels as a Function of Time with a Mobile Analyser
• Nanoporous Carbon from Corn Cobs for Adsorbed Natural Gas Application

### Applied Mathematics in Bioengineering II
***Hilton San Francisco, Continental 4***
• Incorporating Cell Cycle Progression and Drug Penetration into Metabolic Models of Multicellular Tumor Spheriod Growth
• Grey-Box Stochastic Modeling of a an Enzymatic Reactions Network for Biotransformation
• CFD Modeling of Blood Flow in Artery Stenosis
• Utilization of Model Discrimination Analysis in the Description of Bacteriophage Ms2 Viral Dynamics
• A Computational Approach to Identify Optimal Interventions to Bacterial Metabolism
• Model Prediction of Oral Bioavailability of Salt-form Drug Administered with Cyclodextrins: Comparison with in Vitro and *in Vivo* Experiments
• Optimal Treatment of HIV Primary Infection Via a Stochastic Formulation
• Network Biology: from Mechanism-Based Drug Design to Patient Stratification

### Biosensors II: Optical and Implantable Devices
***Hilton San Francisco, Sutter***
• Quantification of Fv and Fvl in Plasma by Using Fiber-Optic Sensing System
• A Novel Nonfouling Poly(Carboxybetaine) Grafted Surfaces with Active Protein Immobilization Groups for Biosensor Applications
• Non-Invasive Determination of Astaxanthin and Chlorophyll in Haematococcus Pluvialis
• Novel Subsecond Voltammetric Separation between Neurotransmitter Molecules in the Presence of Ascorbate
• Engineering Analysis and Modeling of Transport and Catalysis in a Continuous Implantable Biosensor for Lactate and Oxygen Concentration: Investigations with a Membrane-Covered Von Karman Spinning Disc
• In Vivo Monitoring of Tissue Mechanical Properties during Wound Healing
• Insight the Rational Design of Molecularly Imprinted Polymer for the Development of Biomimetic Receptors

### Chemical Vapor Deposition I
***Hilton San Francisco, Powell***
• Knudsen Permeability of Fibrous Films
• Generalized Design Criteria for Vertical Chemical Vapor Deposition Reactors
• Growth and Characterization of Sic Films Deposited in a Large-Scale LPCVD Reactor
• Chemical Vapor Deposition Growth and Characterization of Amorphous, Phosphorous-Doped Ruthenium Films
• Rapid Synthesis of Dielectric Films by Microwave Assisted CVD
• Metalorganic Chemical Vapor Deposition of Ingaasn Using Dilute Nitrogen Trifluoride and Tertiarybutylarsine
• MOCVD Heterostructures of Tio2 and Al2o3 Using Cycling of Tdeat, Tma and O2

### Computational Biology: Membrane Phenomenology
***Hilton San Francisco, Union Square 17 & 18***
• Molecular Dynamics Simulations of Asymmetric Phospholipid Bilayers with Supra-Physiological Transmembrane Potentials
• Investigating Membrane Heterogeneities with Fluorescence Energy Transfer
• The Design of New Protegrin-like Antimicrobial Peptides: a Molecular Dynamics Study
• Disaccharide Binding in Lactose Permease of *E. Coli*: Sugar Structure Influences Binding
• Computational Insights into the Interaction of Non Steroidal Anti Inflammatory Drugs with Lipid Membranes
• Biomembrane Deformations: Molecular Modeling of Key Elastic Properties for Inhomogeneous Lipid Bilayers
• Studying the Human Intestinal Mucin (Muc2) Using Molecular Modeling Approaches for Drug Transport Study
• Relative Binding Free Energy Calculations of Antimicrobial Peptides in Sds/Dpc Micelles Using Molecular Dynamics/Continuum Methods

### Computational Catalysis II
***Hilton San Francisco, Franciscan A***
• Investigation of Nitric Oxide Oxidation Catalysis on Pt(111) Using Density Functional Theory
• A DFT Study of the Structure of Isolated Molybdena Species Supported on Silica and Their Activity for Methane Oxidation to Formaldehyde
• A First Principles Analysis of the Activation of Propane over Substituted Heterpolyacids
• A Quantum-Mechanics/Molecular-Mechanics Study of Potential Steps in Direct Propylene Epoxidation Using $H_2$ and $O_2$ on Au/Titanium-Silicalite-1 Catalysts
• Pseudomorphic Monolayer Catalysts for Denox Applications
• Coverage Dependent Adsorption Energies of Oxygen on Ag-Pd Alloy Surfaces
• Spectral Reconstruction of in Situ Drifts Spectroscopic Reaction Data Using Band-Target Entropy Minimization (BTEM): Application to Nitric Oxide and Carbon Monoxide Adsorption on an Alumina-Supported Platinum Catalyst

### Control of polymorphism of APIs or broader value-added materials
***Hilton San Francisco, Yosemite B***
• Effective Evaluation of Solid-Phase Free Energies
• Impact of Phase Split Ratio on Agglomeration Behavior in an API Crystallization
• Investigation on Polymorphic Transformations of API Using Raman Spectroscopy
• The Kinetics of L-Glutamic Acid Precipitation: Characterization and Modeling
• Polymorphism in the Crystallization of Glycine
• Direct Growth of Gamma Glycine from Neutral Aqueous Solutions by Slow, Evaporation-Driven Evaporation

### Design, Analysis and Operations under Uncertainty II
***Hilton San Francisco, Continental 1***
• A Methodology to Integrate Process Design and Process Control for Chemical Processes
• A Multistage Stochastic MINLP Model for Exploration and Planning of Petroleum Fields under Uncertainty
• Multiperiod Planning of Refinery Operations under Market Uncertainty
• Identification of Hybrid Systems with Application to Fault Detection of a Reverse-Flow Reactor System
• Performing Integrated Process and Control Design Using a Modified Polynomial Chaos Expansion (MPCE) in Optimization under Uncertainty (Ouu)
• Robust Scheduling of Crude Oil Operations under Demand and Ship Arrival Uncertainty
• Integrated Design and Control of Polymerization Reactor under Uncertainty

### Development of Intermolecular Potential Models
***Hilton San Francisco, Union Square 15 & 16***
• Development of Intermolecular Potentials for Thiophenes
• Development of an Opls-Aa Style Forcefield for Polythiophenes
• Effect of Partial Charge Parameterization on the Phase Behavior of Dimethyl Ether
• Application of the Trappe Force Field to the Prediction of Solubility Parameters and Miscibilities
• A Parameterization of the Generalized Born Model for Simulations with Only Torsional Degrees of Freedom
• Calibration of Chemical Bonding in Organo/Metallic System: Interaction between Benzenedithiolate and Gold
• Force Fields for Layered Silicates and Metals
• Molecular Simulation of Propane-Propylene Binary Adsorption Equilibrium in Zeolite 4a
• On the Development of Intermolecular Potentials for Coarse-Grained Models

### Experimental Verification of Multiphase Reaction Engineering Models
***Hilton San Francisco, Franciscan B***
• Multiphase Microreactors - Synthesis and Scaling
• Experimental and Theoretical Explorations of Weak and Strong Gradient Magnetic Fields in Chemical Multiphase Processes
• Multiple Hydrodynamic States in Trickle Flow: Correlating Pressure Drop and Liquid Holdup
• A Combined Experimental and Computational Study of Flow Regimes in a Spout-Fluid Bed
• From Simple Lubrication Models to Industrial Multiphase Monolith Reactors
• Singlet-Oxygen Generation Via Microscale Trickle-Bed Reactor Array: Experiments and Modeling

### Green Materials: Forest and Biobased Products II
***Hilton San Francisco, Union Square 22***
• Microcellular Injection Molding of Polylactide and Polylactide-Montmorillonite Nanocomposites
• Hierarchical Truly Green Nano-Biocomposites Based on a Nano Structure Controlled Bioplastic
• Fiber-Reinforced Composite Foam
• Amylopectin-Clay-Microfibrillar Cellulose Composite Films
• Natural Fibre Reinforced Cellulose Nanocomposites
• Panel Discussion

### Industrial Applications of Computational Chemistry and Molecular Simulations I
***Hilton San Francisco, Union Square 19 & 20***
• Applications of Computational Chemistry and

Molecular Simulation for Product Development at 3M Company
• Modeling Elementary Reactions in Coke Formation from First Principles
• Carbon Cluster Formation during Thermal Decomposition of Energetic Materials HMX and TATB: a Reactive MD Study
• Molecular Simulation Studies on Adsorption of Hazardous Air Pollutants –Hydrogen Cyanide and Methyl Ethyl Ketone
• A Density Functional Theory Study of the Adsorption and Reaction of Co, CH3OH and O2 with Cu-ZSM5, Cu-Y, and Cu-MOR
• Adsorption Phenomena of Mercury-Chlorine Species on a Novel Sorbent Derived from Paper Waste
• Application of Computational Chemistry to the Aqueous Phase Oxidation of Hydroxylamine by Nitric and Nitrous Acids

**Mixing and Chemical Reaction**
***Hilton San Francisco, Union Square 23***
• Local Structure of a Reactive Flow Field on Miscible Viscous Fingering with Chemical Reaction
• A Continuous-Jet Hydrate Reactor for Ocean Carbon Sequestration: Laboratory and Field Experiments
• Hydrogenation in a Stirred Reactor: Simultaneous Bubble Size and Reaction Rate Measurement
• Predicting the Progress of Diffusively Limited Chemical Reactions in the Presence of Chaotic Advection
• Investigation on an Iodine-Iodate Reaction System for Stable Chemical Analysis of $I_3^-$ Ion and Its Application to Characterizing Micromixing Efficiency of a Rotating Disk Reactor
• Interpretation of the Bourne Segregation Parameters for Serial Competitive Reactions

**Modeling for PAT**
***Hilton San Francisco, Union Square 1 & 2***
• Cutting the Gordian Chemometrics Knot – Advantages of the New Method of Sciencebased
• Development of a Process Signature for Fluid Bed Drying Using NIR Spectroscopy
• On-Line Estimation of Diastereomer Composition Using Raman: Differentiation in High and Low Slurry Density PLS Models
• Engineering Considerations on Modeling for Pharmaceutical Process Analytical Technology (Pat) Applications
• Theory of Sampling (ToS) - the Missing Link for Process Analytical Technologies
• Feedforward Modeling Approach to Particle Size Control in Milling Operations
• Development of Protocol for Structure-to-Properties Studies of Non-Platinum Electrocatalysts by Multivariate Analysis and Modeling of Xps Spectroscopic Data

**Nanomaterials: Development, Application, and Societal Impacts on Sustainability**
***Hilton San Francisco, Continental 5***

**Nanoscale Structure in Polymers IV: Polymer Nanocomposites**
***Hilton San Francisco, Plaza A***
• Morphology and Properties of the Rubber Toughened Nylon 6 Nanocomposites
• Modeling and Measurement of Rheological Properties of Poly(Lactide Ethylene Oxide Fumarate)/Hydroxyapatite Nanocomposites
• Preferential Association of Segment Blocks in Polyurethane Nanocomposites
• Atomistic Simulations of Transport of Gas Molecules in Polymer/Nanoporous Inorganic Layered Nanocomposite Membranes
• Polymer Latex/Single-Walled Carbon Nanotube Composites
• The Production and Properties of Exfoliated Polyethylene-Clay Nanocomposites

**Novel Electrochemistry and Materials for Fuel Cells III**
***Hilton San Francisco, Continental 8***
• Ionic Cluster Morphology of Sulfonated Polyarylenethioethersulfone Copolymer Membranes for Fuel Cell Application
• Lattice-Strained Pt Shell Nanoparticle Catalysts
• Development of Novel Pt-Co Catalysts for PEM Fuel Cells
• Polyaniline Nanofibers Supported Platinum Electrocatalysts
• Design of Ordered Catalyst Layers for Polymer Electrolyte Membrane Fuel Cell Cathodes

**Pretreatment of Lignocellulosic Biomass and Interactions with Other Processing Steps II**
***Hilton San Francisco, Continental 7***
• Adsorption and Desorption of Cellulase, Beta-Glucosidase, and Bsa Protein on Pretreated Corn Stover, Cellulose, and Lignin
• Improving Biomass Conversion by Better Fundamental Understanding of Pretreatments: the Case of Ammonia Fiber Explosion (?F??)
• A Novel Ionic Liquid Pretreatment Strategy to Achieve Enhanced Cellulose Saccharification Kinetics
• Factors Affecting the Enzymatic Digestibility of Dilute Acid Pretreated Corn Stover
• Alternative Low-Cost Process for the Hydrolysis of Lignocellulosic Materials for Bioethanol Production
• Understanding the Interactions between T. Reesei Cel7a and the Plant Cell Wall Cellulose Substrate
• Novel Cellulose- and Organic- Solvents-Based Lignocellulose Fractionation: an Update

**Process Engineering of Biobased Products, Paper and Forest Products**
***Hilton San Francisco, Union Square 21***
• Filler Modification for New Paper Product Design
• Permeability and Compressibility of Fiber Mats
• Particle - Bubble Interactions in Flotation Deinking
• Tar and Particulate Removal from a Novel Gasification Unit Using Sawdust as a Feedstock
• Kinetics of Oxygen Delignification from CSTR and Batch Reactor Data
• Process Design Considerations When Selecting a Black Liquor Gasifier

**Process Intensification**
***Hilton San Francisco, Taylor***
• A New Approach to Energy Efficient Process Design
• Heat and Power Optimization in Ammonia Plant
• Effects of Relative Volatility Ranking to the Design of Reactive Distillation
• Multi-Feed Attainable Region Construction
• Process Debottlenecking: Integrated Techniques for Targeting and Design
• Process Intensification Using Novel Micro-Structured Heterogeneous Contacting Systems

**Process Modeling and Identification II**
***Hilton San Francisco, Union Square 14***
• Guaranteed Nonlinear Continuous-Time State Estimation
• Modeling for Reproducible/Optimizing Operation of Fed-Batch Processes
• Parameter Identification for Cybernetic Models of Bioprocesses
• Low-Order Linear Dynamic Models for Prediction of Blood Glucose Concentration
• Modular Design of Nonlinear Observers for State and Disturbance Estimation
• An Ontology Based Approach for Managing General Recipes in Batch Processes
• A Generalized Profiling Approach to Inference Analysis in System Identification

**Product Design**
***Hilton San Francisco, California Room***
• Selection of Solvents for Reactions: a Computer-Aided Methodology with Robust Design Criteria
• A Novel, Systematic Method for Visual Molecular Design
• Proactive Product Quality Control: Bridge the Gap between Theoretical Advancement and Industrial Practice
• Engineering Wine
• Development and Feasibility of a Variable-Area, Sonic Nozzle Mass Flow Controller
• Optimal Design and Layout of an Immunoassay on a Chip

**Solid Dosage Form Design - Formulation and Process Development**
***Hilton San Francisco, Imperial B***
• Modeling and Monitoring of Tablet Bed Dynamics in a Side-Vented Pan Coater by Digital Video Imaging and Analysis
• Assessment of the Segregation Potential of Pharmaceutical Direct Compression Blends
• Scaling Criteria in High Shear Granulator – Empirical Factors Defining Granulation Endpoint
• An Ontology Based Approach for Knowledge Modeling in Pharmaceutical Product Development
• Stable Protein Nanoparticles Produced by Rapid Freezing Processes
• Spray Drying Cellular Material for Long Term Storage
• A New Technology for Pulmonary Drug Delivery
• New Spectrophotometric Method for the Determination of Ambroxol Hydrochloride Using Artificial Neural Networks

**Synthesis and Materials Design**
***Hilton San Francisco, Union Square 3 & 4***
• Organic Electronics: New Materials and Strategies for High Performance Organic Light Emitting Diodes, Thin Film Transistors and Photovoltaic Cells
• Organic Semiconducting Nanostructures Obtained by Self-Assembling Processes: a Scanning Probe Microscopy Characterization
• Texture Changes in Liquid Crystalline Physical Gels
• Synthesis-in-Place of Oligothiophene Micro- and Nano-Patterns Via Photo-Induced Ullmann Coupling Reactions
• Synthesis, Characterization, and O F E T Performance of Functionalized Pentacene Derivatives
• Phenoxazine-Based Organic Semiconductors for Light-Emitting Diodes and Thin Film Transistors

**Systems Engineering Approaches in Biology I**
***Hilton San Francisco, Yosemite A***
• A Novel Optimization-Based Clustering Approach and Prediction of Optimal Number of Clusters: Global Optimum Search with Enhanced Positioning (EP_GOS_Clust)
• Model Predictive Discrimination Approach for Classification of Process and Biological Data
• A Bi-Level Optimization Approach for the Productivity and the Thermodynamic Performance in Metabolic Systems
• Metabolic Flux Elucidation for Genome-Scale Models Using $^{13}C$ Labeled Isotopes
• Identifying the Interacting Residues of a Protein Using Machine Learning: a Case-Study on Fluorescent Proteins

• Elucidating Intracellular Control Mechanisms in Programmed Cell Death

**Tissue Engineering: Bioreactor Studies**
***Hilton San Francisco, Union Square 25***
• Expansion of Human Embryonic Stem (Hes) Cells in a Perfusion Fibrous Bed Bioreactor
• Micro-Bioreactors for 3d Cultures of Human Embryonic Stem Cells
• Propagation of Embryonic Stem Cells without Loss of Their Pluripotency in a Stirred-Tank Bioreactor
• Flow Perfusion Culture of Marrow Stromal Cells on Electrospun Polycaprolactone Scaffolds
• Characterization of Oscillating Flow Perfusion Seeding of RGD-Modified, 3-D Scaffolds with Mesemchymal Stem Cells
• Endothelialization and Flow Conditioning of Fibrin-Based Media-Equivalents
• Application of Biochemical and Biophysical Stimuli to Bone Marrow-Derived Stem Cells with Aims for Functional Ligament Tissue Engineering

**Topics in Surface Science and Catalysis II, In Honor of Robert J. Madix**
***Hilton San Francisco, Imperial A***
• Catalytically Active Gold: from Nano-Particles to Ultra-Thin Films
• Towards an Understanding of Surface Electrochemical Reaction Kinetics
• Photocatalytic Decomposition on Pt/Tio2
• Thermodynamics of Surface Reactions: Relationship to Reactivity
• Oxidation of Pt Surfaces with Gaseous Oxygen Atoms
• Above the Transition: Methane Oxidation on Metallic Palladium at 10-Atm
• Structure of Surfaces in Equilibrium with Low and High Pressure Gas Environments

**FRIDAY, 17 NOVEMBER 2006**
***3:15 PM - 5:45 PM***
**(22c) Nanowires IV: Applications of Nanowires**
***Hilton San Francisco, Plaza B***
• A 160 Kbit Molecular Electronic Memory Circuitry at 10^11 Bits/CM^2
• Aligned and Oriented Polyaniline Nanofibers
• Aluminum Nanowire Polarizing Grids Via Block Copolymer Lithography: Fabrication and Analysis
• Nanowire Based Dye Sensitized Solar Cells and Electrochromic Devices
• One-Dimensional Nanostructures as Subwavelength Photonic Elements
• Single Crystal InSb Nanowires: Synthesis, Characterization, Properties and Applications

**Advances in Cell Culture and Bioreactors**
***Hilton San Francisco, Imperial B***
• Optimization of in Vitro Erythropoieis for Genotoxicity Testing
• Model-Based Optimization of Mammalian Cell Cultures: a Case Study for Optimizing Glucose and Glutamine Fed-Batch Profiles for CHO-IFN$\gamma$ Cell Line
• Liver Endothelial Cells Promote LDL-R Expression and the Uptake of Hcv-like Particles in Primary Hepatocytes
• Insights into Hepatic Metabolism from Flux Balance and Pathway Analyses
• Engineering Cancer-Specific Cis-Acting Intronic Regulators of Alternative Splicing as Novel Tools for Disease Detection and Treatment
• Effects of Igf-1 Modified EHD Networks on Myoblastic Cell Proliferation
• Comparison of Gene Expression Systems for Production of Recombinant Human Therapeutics in Transgenic Plant Cell Cultures

**Application of engineering fundamentals to API process development - PAT applications**
***Hilton San Francisco, Yosemite B***
• Applications of Process Analytical Technologies to Ensure Controlled Processes
• Selective Crystallization of the Metastable Alpha Form of L-Glutamic Acid through Feedback Concentration Control
• Using Continuous Integrated Micro Filtration for the Production of Pseudotype Vectors in a Fixed Bed Reactor
• Mapping the State of a Pharmaceutical Co-Precipitate Process: an Integrated Process Analytical Technology (Pat) Approach
• Understanding Primary Atomization in Sprays
• A.P.I. Crystal Engineering in Early Development

**Atomic Layer Deposition**
***Hilton San Francisco, Powell***
• Process – Structure Relationships of $Al_2O_3$ and $HFO_2$ Composite Films on Silicon
• Quantum Molecular Dynamics Simulations of the ALD of HFO2
• Spatially Controlled Nano-Scale Doping by Atomic Layer Deposition
• Modified Titania Films for Photoelectrochemical Applications
• Kinetics of ALD Ruthenium Nucleation and Growth Studied Using on-Line Auger Electron Spectroscopy
• Material and Electrical Properties of HF-Ru-N Gate Electrodes on Hafnium Oxide
• Lithography Via Top Surface Imaging Using Area Selective Atomic Layer Deposition

**Biosensors III: Saw Devices and Sensor Development**
***Hilton San Francisco, Sutter***
• Binding Kinetics of Free and Total Specific Prostate Antigen Using Fractal Analysis
• Fractal Analysis of Heparin-Protein Interaction Studies Occurring on Biosensor Surfaces
• Simultaneous Surface Manipulation and Sensing in a Biosensor Using a Hexagonal Saw Device
• Finite Element Modeling of Acoustic Streaming in Surface Acoustic Wave (Saw) Devices
• Development and Characterization of Antibody Molecules on Peg Tethered Aln-Based Biosensors
• Treatment of Aluminum Nitride Biosensor Surfaces for Improved Silanization
• Development of an Amperometric Sensor for Chiral Recognition in Organic Solvent Using the Gate Effect of Molecularly Imprinted Polymer
• Micro-Chameleons: Nonlinear Chemical Microsystems for Amplification and Sensing
• Fractal Binding and Dissociation Kinetics of Heart-Related Compounds on Biosensor Surfaces

**Chemical and Catalytic Conversions and Processes for Renewable Feedstocks**
***Hilton San Francisco, Continental 7***
• Transesterification of Poultry Lipids Using Mg-Al Hydrotalcite Derived Catalysts
• Preliminary Investigations of the Catalytic Deoxygenation of Fatty Acids
• The Effects of Temperature and Hydrogen on Glycerol Adsorption on Ruthenium Metal
• In-Situ X-Ray Absorption Spectroscopy of Supported Transition Metal Catalysts for Hydrogenolysis of Sorbitol and Oxidation of Glycerol
• Highly Selective Conversion of Glycerol to Propylene Glycol
• A New Route to Improved Glucose Yields in Cellulose Hydrolysis

**Computational Catalysis III**
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• A Reaction Mechanism for the Nitrous Oxide Decomposition on Binuclear Oxygen Bridged Iron Sites in Fe-ZSM-5