

Paper Number	Paper Title	First Name	Last Name	Affiliation
7n	Computational and Experimental Investigation of Membrane Biomechanics	Manuela A.A.	Ayee	University of Illinois at Chicago
7w	Computationally Driven Discovery of Novel Materials for Separation and Catalysis	Peng	Bai	University of Minnesota
7o	Machine Learning and Molecular Dynamics Map Conformational Landscape of $\mu$ -Opioid Receptor	Amir	Barati Farimani	
7c	Solubility and Thermodynamic Properties of $\alpha$ -Amino Acids in a Model System of Industrial Residues	Nathan	Bowden	
7e	Reverse Engineering of Molecular Structure	Farhad	Gharagheizi	
7k	Computational Soft Matter	Jens	Glaser	University of Michigan
7d	Exploring Fundamentals of Zeolite Catalysis – a Theoretical Perspective	Florian	Görtl	UW Madison
7a	Computational Methods for Predicting and Understanding Chemical Reactivity: Catalysis, Biology, and Beyond	Joseph S.	Gomes	University of California Berkeley
7v	Quantitatively Reliable Molecular Modeling and Simulation of Vapor-Liquid Equilibria	Martin	Horsch	University of Kaiserslautern
7i	Enhanced Molecular Simulations for Applications in Protein Stabilization, Crystallization, and Structural Determination	Vance	Jaeger	Max Planck Institute for Biophysical Chemistry
7u	Computationally Assisted Discovery of Well-Designed Materials for Applications to Energy, Environment, and Catalysis	Ki Chul	Kim	Georgia Institute of Technology
7l	Design and Discovery of Multifunctional Nanoporous Materials	Ambarish R.	Kulkarni	Georgia Institute of Technology
7h	Modeling Chemical Reactivity for Nanoscale Design	Ryan Gotchy	Mullen	University of California
7b	Towards Accurate Atomistic Description of Reactive Interfaces for <i>in silico</i> design of Novel Functional Materials	Badri	Narayanan	Argonne National Lab
7q	New Generation of Polarizable Reactive Force Fields for Multiscale Simulations of Complex Materials	Saber	Naserifar	California Institute of Technology
7j	Advanced Materials Design Using Molecular Simulation, Evolutionary Computing and Machine Learning	Tarak Kumar	Patra	The University of Akron
7t	Accelerating Materials Design: Computer Simulations and QSAR Modeling	Qing	Shao	North Carolina State University
7x	Flexible and Dynamic Porous Crystals	Cory	Simon	
7g	Simulation of Selectively Permeable Novel Polymeric Membranes	Marielle	Soniat	
7f	Developing Molecular Theories/Simulations to Understand and Optimize Soft Matter Systems: From Ions to Polymers to Gels	Rui	WANG	California Institute of Technology
7s	Software Engineering for the Molecularly Minded	Frank T.	Willmore	National Institute of Standards and Technology
7p	Towards More Rational Design of Electrocatalyst for Carbon Dioxide Reduction	Jianping	Xiao	
7m	Hydrodynamic Model of Complex Liquids with Microstructure	Rui	Zhang	CCNY
7r	Dispersion-Corrected Density Functional Tightening Binding Modeling of the Natural Metastable Twin Boundary of Organic Energetic Materials: Beta-Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine	Liu	Zhichao	China University of Petroleum