



The Western Palmetto Informer

American Institute of Chemical Engineers

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~~February 11, 2014~~ changed to February 18, 2014

Molecular Modeling & Computer Simulations in Materials Engineering

In This Issue

- Next Meeting:
~~February 11th~~
February 18th
- Upcoming 2014 Events
- Officers and Executive Committee
- Clemson Scholarship

An ability to design materials molecule-by-molecule is the Holy Grail of materials science and engineering. Molecular modeling and computer simulations, in principle can be powerful tools to this end. They can provide an economical route to screen through hundreds of thousands of molecules for desired properties. In this talk, Dr. Sarupria, Clemson University professor, will give a brief introduction to molecular modeling and computer simulations and provide some examples of how these can provide fundamental insights into materials properties. She will talk about two projects - one from the field of biology - indicating how simulations can help understand protein stability and function; and the second related to on-going work on dendritic polymers and their development of water purification applications.

Dr. Sarupria received her B. Tech degree from Chaitanya Bharathi Institute of Technology in Hyderabad, India, M.E. degree from Texas A&M University, College Station, and Ph. D. degree from Rensselaer Polytechnic Institute, all degrees in Chemical Engineering.

She was a postdoctoral researcher at Princeton University before joining Clemson University in Spring 2012. She received the Award of Excellence in Computing Research from the American Chemical Society Chemical Computing Group in 2008, and the best poster awards at Gordon Research Conference in 2007 and 2010.

Dr. Sarupria's research focuses on studying problems relevant to bioengineering, energy and environment at the molecular level using molecular modeling and computer simulations. Her current work involves understanding liquid-to-solid transitions in aqueous systems, specifically nucleation of ice and gas hydrates, and developing computationally viable models to study the biological self-assembly and polymeric systems. She currently has 2 graduate students and 5 undergraduate students in her research lab. We look forward to seeing you there!

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February Meeting Information

TITLE: Molecular Modeling and Computer Simulations in Materials Engineering

DATE: Tuesday, February 11, 2014

TIME/PLACE: Hilton on Haywood Road
6:00 PM Social
6:30 PM Dinner
7:00 PM Presentation

DIRECTIONS: I-85 to I-385 N towards Greenville
Exit 35, Haywood Road
TURN Right off of exit ramp,
TURN Left at first light (have to cross 3 lanes of traffic)
Hotel is on the left behind/next to the Bank of America
(toward east end of stadium)

COST: \$10 for Members, \$15 for Non-members
No cost to Attend Presentation without dinner

Three ways to RSVP by 2PM - Friday, February 7th, 2014

Old fashioned phone call to Secretary - Conny Walker (864) 483-2920

Turn-of-the-century email to the same at sec@wscaiche.org

Modern Facebook APP Event - [February WSC AIChE Facebook Event](#)

Clemson Scholarship to be Awarded

The Executive Committee has again agreed to support Clemson's Chemical and Biomolecular Engineering program with a \$1,000 scholarship. The candidate has been selected and will be awarded at the February 2014 chapter meeting.

Science & Engineering Fair Support Continues

Our section will continue to assist in judging student projects and providing monetary awards at the South Carolina Regional Science & Engineering Fair in 2014. Please contact Conny Walker, at sec@wscaiche.org if your company is interested in sponsoring judges or special awards for this endeavor.

2014 Upcoming Events

DATE	LOCATION	TOPIC
11 Feb 2014	Greenville Hilton	TBA - Clemson University Provided Speaker
11 Mar 2014	FUJIFILM Greenwood, SC	Plant tour - FUJIFILM Water Recycling System
Mar 2014	TD Convention Center	Science Fair Judging for the Greenville County Science Fair
08 Apr 2014	ASHLAND, INC. Piedmont, SC	Plant tour - ASHLAND
May 2014	TBD	Family Social

2013-2014 Officers and Executive Committee

This is YOUR local section of the American Institute of Chemical Engineers. Please contact any Officer or Executive Committee member listed below with your suggestions, ideas and/or concerns.

POSITION	NAME	EMAIL	PHONE
Chair	Rick Vogel	rvogel1@hotmail.com	864-420-5777
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