“Functional Materials by Design”

Saurabh Ghosh
Vanderbilt University, Nashville, TN
Host: Ward Plummer

3:30 PM Thursday, February 2, 2017
119 Nicholson Hall

• Refreshments served at 3:10 PM in 232 (Library) Nicholson Hall •

The Density Functional Theory (DFT), which is a first principles method, has been the governing method for quantum mechanical simulation of materials for the past 30 years. Using this theory structural, electronic, magnetic and other properties of a many electron system can be determined. With the advancement of modern supercomputing capabilities, DFT is not only successful in explaining experimental findings but also predicting materials with new functionalities. Understanding the ‘structure-property’ relationship of a material is the key to designing new functionality. This colloquium will discuss ‘structure-property’ relation of functional materials based on DFT calculations, guided by group theoretical techniques, and supported by phenomenological modeling. The focus will be on functional materials that impact energy, and electronics.

Publications

• “Evolution in totally constrained models: Schrödinger vs. Heisenberg pictures” by Javier Olmedo
LSU Physics & Astronomy in the News


Events

- **Saturday Science**: “The Science of Deepwater Horizon Oil Spill” by Emily Mauna-Douglass from Louisiana Sea Grant College  
  **When**: 10-11 AM Saturday, January 28, 2017  
  **Where**: Room 130 Nicholson Hall

- **LaCNS seminar**: “Utilizing Coordination-Insertion Based Polymerizations for the Synthesis of Tailored Polyolefins and Gas Separation Membranes” by Brian Long from University of Tennessee Knoxville  
  **When**: Friday, February 3, 2017 12:30 PM  
  **Where**: 208 Williams Hall

- **Landolt Observatory Public Night**: Venus and Mars conjunction  
  **When**: Saturday, February 4, 2017 6:30 PM - 7:30 PM  
  **Where**: Nicholson Hall roof - Landolt Observatory

Please see the attached flyers
The Science of Deepwater Horizon Oil Spill

A public lecture by
Dr. Emily Maung-Douglass

About the Speaker

Dr. Emily Maung-Douglass is an oil spill specialist at Louisiana Sea Grant. Her work, funded by the Gulf of Mexico Research Initiative (GoMRI), focuses on chemical evolution and breakdown of petroleum and dispersants in the environment as well as their interactions with the ecosystem.

Deepwater Horizon oil spill occurred in 2010 off the coast of Louisiana and continues to be the largest accidental release of oil on record. What have scientists discovered about the spill in the past seven years? How are scientists continuing to study the impacts of the spill and preparing for the next one?

Please join us at LSU’s next Saturday Science Lecture to learn the answers to these questions and more!

28 January 2017, 10-11:00 a.m.
Room 130 Nicholson Hall, LSU
Utilizing Coordination-Insertion Based Polymerizations for the Synthesis of Tailored Polyolefins and Gas Separation Membranes

Coordination-insertion based polymerization methods provide a multitude of opportunities for enhanced control over catalytic activity, selectivity, and reactivity. Through tailored catalyst development and macromolecular design, the Long Research Group leverages these advantages to synthesize unique and/or tailored polymeric structures for a variety of applications. In this talk, we will demonstrate the potential power of these coordination-insertion based polymerization methods through two studies. First, we will provide fundamental evidence that redox-active olefin polymerization catalysts can be effectively used to modulate polyolefin microstructure and copolymer composition via simple in situ changes in a catalyst's oxidation-state. Second, we will demonstrate that careful catalyst selection can enable access to a unique class of polymers that was previously believed to be inaccessible, and that those materials are extremely attractive as highly efficient gas separation membranes.