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Department of Physics & Astronomy

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Weekly Calendar

March 30 – April 3, 2015

Departmental Colloquium

"Manipulation of Phonon and Spin Dynamics at the Nanoscale"

3:30 PM Thursday, April 2, 2015

435 Nicholson Hall

Min Quyang
University of Maryland

HOST: Jiandi Zhang

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

"In this talk I will present a few recent advances from my research group, centering on coherent manipulation of fundamental phonon and spin dynamics in precisely engineered colloidal hybrid nanostructures by ultrafast all optical techniques. Ultrafast optical spectroscopy not only offers a unique tool to probe phonon and spin dynamics with extremely high sensitivity but also allows precise control of fundamental quantum processes at the nanoscale. For example, I will demonstrate how to apply ultrafast optical spectroscopy to reveal coherent phonon modulation through nanoscale acoustically mismatched interface. By employing a sequence of coherent laser pulses selective phonon modes can be enhanced or annihilated, and the interplay between different phonon modes can be tailored. Furthermore, ultrafast coherent spin manipulation can be achieved in semiconductor quantum structures through novel plasmon-exciton resonant coupling. This has recently enabled first demonstration of all optical spin echo in colloidal semiconductor nanostructures, with manifestation of intrinsic long spin lifetime. All these together should offer valuable opportunity to reveal nature of quantum phonon and spin couplings at the nanoscale."

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Spring Seminar
John Keith
University of Pittsburgh

"Exploring CO_2 Conversion Into Commodity Chemicals with First Principles Quantum Chemistry"

3:30pm, Wednesday, April 1, 2015

Announcement:

Highland Road Park Observatory

6th ANNUAL
NANO DAYS
Saturday, March 28, 2015 from 2:00 pm to 6:00 pm
No admission fee. For ages six and older.

Publications:

1."Electron-scattering form factors for Li-6 in the ab initio symmetry-guided framework", **T. Dytrych**, A. C. Hayes, **K. D. Launey**, **J. P. Draayer**, P. Maris, J. P. Vary, D. Langr, and T. Oberhuber, Phys. Rev. C 91, 024326 (2015).

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Exploring CO_2 Conversion into Commodity Chemicals with First Principles Quantum Chemistry

– John A. Keith, University of Pittsburgh

SEMINAR
WEDNESDAY
APRIL 1
1008B DMC
LSU
3:30 PM

A key component of human sustainability is the utilization of CO_2 from post-combustion processes. An intriguing avenue is the (photo-)electrochemical conversion of CO_2 into commodity chemicals such as CO, formate, and methanol. Aromatic N-heterocycle (ANH) molecules have been found to promote these reactions, but a mechanistic understanding of how this chemistry occurs is not well understood. This presentation will concentrate on our work identifying calculable pK_a and redox potential descriptors for ANH molecules to help identify which molecules at what experimental conditions would facilitate efficient (photo-)electrochemical conversions of CO_2. We will report our progress in rationalizing possible reaction mechanisms for ANH-promoted processes in light of recent experimental and computational investigations. We will also show applications of nudged-elastic band calculations in tandem with ab initio molecular dynamics simulations for unbiased analysis of CO_2 conversion mechanisms in aqueous solution.

Dr. Keith is an R. K. Mellon Faculty Fellow in Energy, a tenure-track assistant professor, at the University of Pittsburgh (Pitt) in the Department of Chemical & Petroleum Energy and affiliated with Pitt's Center for Energy. After obtaining his Ph.D. from Caltech, he was an Alexander von Humboldt postdoctoral fellow at the University of Ulm and then an Associate Research Scholar at Princeton University. He began his appointment at Pitt in September 2013. His group uses first-principles based computational chemistry to study chemical reaction mechanisms and design materials and catalysts for alternative energy conversion. Current activities address CO2 conversion, homogeneous heterobimetallic catalysis, and atomistic potential development for nanoscale simulations, all with intended applications in sustainability and renewable energy.
http://www.klic.pitt.edu/

All seminars are available via HD videoconferencing at the following venues:
LA Tech - 122 Nethken Hall, LSU - 1008B DMC, SUBR - 211 J.B. Moore Hall,
Tulane - 600 Lindy Boggs, UNO - 234 Liberal Arts Building, Xavier - 226 Qatar Pavilion.

NanoDays at the Highland Road Park Observatory

Saturday, March 28, 2:00-6:00 p.m

It's a Big Celebration of Things that are Too Small to See!

You're invited to an afternoon of free family fun at NanoDays. It's a nationwide celebration of nanoscale science and engineering. Learn how the iridescent colors in butterfly wings are really just tiny patterns that reflect light. Or how tinted glass in old cathedrals was made by mixing different sizes of gold particles. Nanotechnology has so many promising uses, from advanced computer processing and storage, to new medical treatments, and much more.

NanoDays features several hands-on activities for visitors to see, smell, touch and hear.

- Learn first-hand how a Scanning Probe Microscope helps scientists explore the nanoworld
- See how nanomaterials are used to make stain-free clothes
- Play with liquid crystals and magnets
- Make your very own Oobleck.

At 4:00 p.m., get inside the large mind of a "mad nano scientist." Dr. Michal Brylinski, a professor with the LSU Department of Biological Sciences, will discuss "**Computational Biology, Drug Discovery and Video Games.**"

Spend the afternoon with faculty, students and staff from:

- the LSU Center for Computation and Technology;
- the Department of Physics & Astronomy; and,
- the National Science Foundation-funded Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA).

NanoDays *is a nationwide celebration that takes place March 28-April 5, 2015, at more than 200 science museums, research centers and universities across the country. NanoDays is organized by the* ***Nanoscale Informal Science Education Network*** *(NISE Net.).*

For more information, please visit http://lasigma.loni.org or contact Dr. Juana Moreno at moreno@lsu.edu.

LA-SiGMA

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