



College of
Science

Department of Physics
& Astronomy

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Weekly Calendar

May 4 - 8, 2015

Departmental Colloquium

"Implications to High T_c Superconducting Mechanism from Iron-Based Superconductors"

3:30 PM Thursday, May 7, 2015

119 Nicholson Hall

Jiangping Hu

Purdue University

HOST: Rongying Jin

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

The discovery of iron-based superconductors six years ago dethroned the cuprates as the dictator of high T_c superconductors in correlated electron systems and generated great hope and excitement to solve the decades-odd problem of non-BCS (Bardeen, Cooper and Schrieffer) high T_c mechanism. However, the optimism was dying out in the past several years as more iron-based superconductors were discovered and an unified understanding of all materials became increasingly difficult.

In this paper, we take the "top-to-bottom" approach to review and examine both experimental and theoretical results on pairing symmetries of the iron-based superconductors. We argue that the pairing symmetries throughout all families of iron-based superconductors, including both iron-pnictides and iron-chalcogenides, universally belong to A_{1g} s-wave. The s-wave symmetry is robust against doping changes and variations of Fermi surfaces.

The robust s-wave symmetry in iron-based superconductors has even deeper fundamental implications on magnetically driven high T_c mechanisms than the d-wave symmetry in cuprates did. We show that it sets a few important guiding principles to search for new high temperature superconductors.

Special Seminar:

Louisiana Consortium for Neutron Scattering

"Elucidating the Structure-Performance Relationship in Organic Photovoltaics (OPVs) by Grazing Incidence X-Ray Scattering"

Monday, May 4, 2015, 3:00-4:00 pm

1008B Digital Media Center, LSU

Joseph Strzalka

Argonne National Laboratory

Spring Seminar

Neeraj Rai

Mississippi State University

“Modeling Complex Chemical Systems: Insights in Catalytic Activity of Sn-Beta Zeolite and Thermophysical Property Prediction”

3:30pm, Wednesday, May 6, 2015

211 Nethken Hall, LA Tech

Announcements:

Saturday Science @ LSU

“Vibrations and resonance in network graphs”

May 2, 2015

10:00 – 11:15 AM, Room 130 Nicholson Hall

**Stephen Shipman
LSU, Dept. of Mathematics**



Monday, May 4
3:00-4:00pm
1008B Digital Media Center
Louisiana State University

Elucidating the Structure-Performance Relationship in Organic Photovoltaics (OPVs) by Grazing Incidence X-Ray Scattering

Since the introduction of the Bulk Heterojunction (BHJ) architecture in the mid 90s, organic photovoltaic devices have made steady progress toward improved power conversion efficiency, and are now poised to move from niche products to large scale commercial applications. In the BHJ, the photoactive layer consists of electron donor and acceptor materials in a bicontinuous phase blended on the nanoscale. Grazing incidence x-ray scattering, capable of characterizing thin film nanomorphology of surfaces and interfaces, has emerged as a key technique for investigating OPV materials. The hierarchical variety of lengthscales present in OPV materials requires both grazing incidence small- and wide-angle x-ray scattering, the latter recently enabled by improvements to the GISAXS instrument at 8-ID-E of the Advanced Photon Source. I will describe grazing-incidence studies at 8-ID-E that have contributed toward unraveling the complex relationship between OPV materials, processing and performance.

SEMINAR SERIES 2015



Guest Speaker

**JOSEPH
STRZALKA**

Assistant Physicist,
Time Resolved
Research

X-ray Science Division
Argonne National Lab

Dr. Strzalka's research interests include proteins at interfaces, organic photovoltaics, grazing incidence x-ray scattering, and liquid surface scattering. He earned his PhD in Physical Chemistry and MS in Physics at the University of Pennsylvania.

Free and open to the public



www.physics.lsu.edu/lacns



Modeling Complex Chemical Systems: Insights in Catalytic Activity of Sn-Beta Zeolite and Thermophysical Property Prediction

– Neeraj Rai, Mississippi State University



**SEMINAR
WEDNESDAY
MAY 6
211 NETHKEN HALL
LA TECH
3:30 PM**

Computational science is now widely recognized as the third pillar of scientific enquiry. Algorithmic improvements coupled with advances in computer hardware allow us to investigate more complex systems with greater detail. In this talk, I will present an application of electronic structure calculations to explore catalytic activity of Sn-Beta zeolite for isomerization and epimerization of glucose. Glucose to fructose isomerization is a key step in the conversion of biomass to chemicals. A better understanding of zeolitic activity for this reaction can allow us to develop more efficient catalyst for biomass conversion. In the second half of the talk, I will discuss Monte Carlo algorithmic improvements that allowed us to compute vapor liquid equilibria of ionic liquids using atomistic force fields, and discuss the suitability of dispersion corrected density functionals in predicting the phase equilibria of hydrofluoromethanes.

Neeraj Rai obtained bachelor's degree in Chemical Engineering from Karnataka Regional Engineering College, Surathkal, India in 2000. After short industrial stint in a fertilizer plant (Ammonia/Urea complex), he pursued his research interests first at Indian Institute of Science, Bangalore and later at the University of Minnesota, where he obtained PhD degree in Chemical Physics in 2009. Subsequently, he performed postdoctoral work at the University of Notre Dame and the University of Delaware. In August 2013, he started as an Assistant Professor in the Dave C. Swalm School of Chemical Engineering at Mississippi State University. His research interests are in the areas of force field and algorithm development, catalysis, and self-assembly of organic molecular systems. <http://railab.che.msstate.edu/>

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