LSU College of Science Department of Physics & Astronomy

202 Nicholson Hall
Louisiana State University
Baton Rouge, LA 70803
TEL: 225-578-2261
FAX: 225-578-5855
http://www.phys.lsu.edu

Weekly Calendar

April 16 – April 22, 2016

Departmental Colloquium

" Surely You're Joking Mr. Feynman, When You Say Materials Design is Fundamental Physics"

3:30 PM Thursday, April 21, 2016
109 Nicholson Hall

Craig Fennie
Cornell University

Host: Ilya Vekhter

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

Today, first-principles quantum techniques are powerful tools for analyzing and interpreting the properties of crystalline materials, yet the theoretical design of new materials with targeted properties remains challenging. Why? At a fundamental level, the laws governing the physics of materials are in fact relatively simple; it is just that the behavior of the constituents as a whole is complex. Indeed, materials are made up of atoms whose type, number, and arrangement - the crystalline motif - creates distinct properties that emerge through the collective behavior of the seemingly simpler, well-understood parts. The discovery of emergent phenomena in condensed matter systems is therefore intimately linked with that of discovering the crystalline materials that display these phenomena. Such discoveries by their very nature often occur serendipitously, which appeared to have annoyed Richard Feynman enough for him to make a bold, often forgotten, statement on the subject.

In this talk I will provide my interpretation of his statement, how it relates to the recent White House "Materials Genome Initiative", and will discuss our theory-driven approach to help change the situation, highlighting the challenges. Our modus operandi combines microscopic Hamiltonians/models with fundamental principles of solid-state chemistry and first-principles simulations. For example, using the perovskite ABO3 complex oxides as a materials platform, I will show how we think about manipulating the atomic scale structure to control the interplay among the active charge/orbital, magnetic and electronic degrees of freedom so as to produce "designer" properties and functionalities such as the electric-field control of magnetism, and possibly, a metal/insulator transition. I will give a very recent example in which we started with a pen & paper to understand the possibility for new physics, used first-principles calculations to discover a class of material realization, and ended with two groups reporting the experiential proof and much more.

LSU Physics & Astronomy in the News

- Long-term observations made with the Gemini Multi-Object Spectrograph at Gemini South, combined with Spitzer space telescope data, reveal how core collapse supernovae can make an important, yet largely unrecognized, contribution to the overall dust budget of the Universe. The research of **Geoff Clayton** with his graduate students, **Kelsie Krafton** and **Ed Montiel**, as well as his former grad student, Jen Andrews, is featured in Gemini Focus this month on pages 5-8. Read more

- Small Science Wields Big Ideas - LSU Celebrates NanoDays: The Biggest Event for the Tiniest of Science. For the seventh consecutive year, LSU will host NanoDays at the Highland Road Park Observatory on Saturday, April 16, from 2-6 p.m. Read more

- Quantitative LEED Analysis Workshop will be held at 1034 LSU Digital Media Center from April 18 to 20 by Dr. Ward Plummer's research group.

New Publications

- **Francois Mauger**, **Paul M. Abanador, Kenneth Lopata, Kenneth J. Schafer,** and **Mette B. Gaarde**. have introduced a semiclassical-wave-function model for strong-field physics and attosecond science and apply it to the analysis and prediction of high-harmonic generation spectra. "Semiclassical-wave-function perspective on high-harmonic generation," Phys. Rev. A **93**, 043815 - Published 11 April 2016.

Landolt Astronomy Observatory Public Observing Night

April 16, 8:30-9:30 PM. Public Observing on the Roof of Nicholson Hall
"Jupiter near gibbous Moon"

NanoDays

2-6 p.m.

Saturday, April 16

Highland Road Park Observatory

The observatory will have this month's solar viewing session from 2:30-4:30 p.m. through HPO's Coronado Solar Max II.

Lunar viewing will take place from 4:30 - 6:30 p.m. showing a magnified daytime moon.

Small Science Wields *BIG IDEAS*

NanoDays 2016

Join LSU for the 7th annual NanoDays at the Highland Road Park Observatory on Saturday, April 16, from 2-6 p.m. The free family-friendly event is open to the public and will feature several hands-on activities for guests of all ages:

- 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 an Oobleck, a liquid with both liquid and solid properties
- At 4 p.m., get inside the mind of physicist Shane Stadler, a professor in the LSU Department of Physics & Astronomy, who will present **"Magnetic Refrigeration: "The New Cool"**

SPONSORED BY:

LSU College of Science Department of Physics & Astronomy

Consortium for Innovation in Manufacturing Materials

LSU Center for Computation & Technology

International Workshop on QUANTITATIVE LEED ANALYSIS

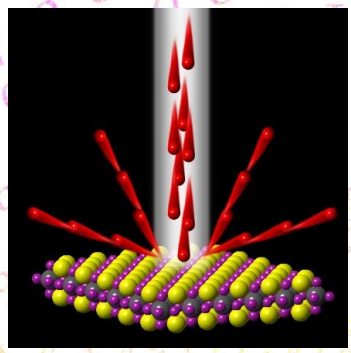
2016
April 18-20
Louisiana State University
Digital Media Center, Rm1034

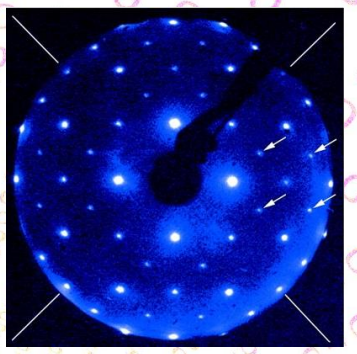
Plenary Speakers:

Prof. John Rundgren
KTH Royal Institute of Technology,
Stochkholm, Sweden

Prof. Von Braun Nascimento
Universidade Federal de Minas Gerais,
Belo Horizonte, Brazil

Prof. Steven Brandt
Louisiana State University,
Baton Rouge, USA.

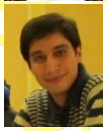




Organizers:

Prof. Ward Plummer
Louisiana State University,
Baton Rouge, USA.

Chen Chen
Louisiana State University,
Baton Rouge, USA.



Mohammad Saghayezhian
Louisiana State University,
Baton Rouge, USA.

Plenary talks:

- **Elastic Electron-Atom Scattering in Solids and Surface slabs**
- **Differential Evolution: Global search Problem in LEED-IV Surface Structural Analysis**
- **Parallelizing Modern Codes with OpenMP, MPI, C++11, and HPX**

Afternoon hands-on workshops

- **Introduction to Linux**
- **Scattering phase shift calculation**
- **Symmetrized automated tensors LEED calculation**

For **registration**, please contact
Chen Chen (cchen22@lsu.edu)
Mohammad Saghayezhian (smoha12@lsu.edu)

LACNS

Louisiana Consortium for Neutron Scattering

SEMINAR SERIES 2016

Monday, April 18
3:00pm
1008B Digital Media Center
Louisiana State University

Dispersion Morphology of Nafion in the Fabrication of Fuel Cell Membrane Electrode Assemblies: Relationships to Electrolytic Fuel Call Durability and Performance

Modern polymer electrolyte fuel cells (PEFCs) require technologies that generate higher performance, durability and component structural integrity. The membrane electrode assemblies (MEAs) of PEFCs typically contain a Pt/carbon black catalyst and an ionomer, such as Nafion. In one process MEAs are produced by solution casting from a dilute solvent dispersion of these components. We consider current hypotheses relating fuel cell durability and MEA toughness to changes in these components with multiple fuel cell voltage potential cycling: namely, that fuel cell durability is associated with the loss of electrochemical (Pt) surface area (ECSA) and that MEA mechanical properties are due to ionomer crystallinity. We weigh these hypotheses against an alternative that both fuel cell durability and MEA toughness are the result of dispersion particle morphology and its evolution during the course of drying to the MEA film. Small-angle neutron scattering (SANS) using the Lujan Center instrument, LQD, was used to show that different solvents determine the dispersion particle structure due to the amphiphilic nature of Nafion and that the morphology of the dispersion in different solvents follow different evolutionary paths on drying. The SANS results suggested that the ability of the dispersion particles to form an entangled network leading to a homogeneous, reversible gel alone was the determining factor for mechanical toughness of the MEA and fuel cell durability. It was found that neither toughness correlated with Nafion crystallinity nor was durability correlated with changes in the ECSA with voltage cycling. These results show the power of SANS as a characterization technique, when used along with other characterization methods and property and performance metrics, to address complex issues in materials science process, structure, properties and performance characteristics. Our work lends support to the hypothesis that MEA durability and toughness are affected by the dispersion morphology and are likely associated with the ability of Nafion to chain entangle.

Guest Speaker

Dr. Rex Hjelm

Instrument Scientist

Los Alamos Neutron Science Center, Los Alamos National Laboratory

Free and open to the public

EPSCoR DEPARTMENT of ENERGY

www.physics.lsu.edu/lacns

LSU LOUISIANA STATE UNIVERSITY · LOUISIANA TECH UNIVERSITY · THE UNIVERSITY of NEW ORLEANS · Tulane University