

**FSMS 2011 Annual Meeting  
Preliminary Schedule  
August 1-2, University of Central Florida**

**Monday August 1, Harris Engineering Center 101**

1:00-4:00pm Presentations by faculty, postdocs, students

1:00-1:30 **Eric W. Bucholz** and Susan B. Sinnott, "*Mechanics of Individual Nanoparticles from Experiment and Simulation*"

1:30-2:00 **Joshua Bush**, Rashmi R. Mohanty, and Yongho Sohn, "*Phase-field Modeling of Thermotransport in U-Zr Alloys*"

2:00-2:30 Break

2:30-3:00 **Patrick K. Schelling** and Zachary McDargh, "*Atomic scale simulation of thermotransport*"

3:00-3:30 **Marisol Alcantara Oritgoza**, "*First-principles clarification of the spin-orbit coupling on Bi(111)*"

3:30-4:00 Poster set up

4:00-5:30pm Poster session

6:30 – 8:30 Dinner – Olive Garden

**Tuesday August 2, Harris Engineering Center 101**

**Surveys, student evaluations (9 AM – 9:30AM)**

9:30-10:00 Schelling, informal discussion– Writing Papers and Proposals

- General advice on improving writing skills.
- Brief discussion on giving good presentations.
- Q/A session – this will be the dominant part of the session.

10:00-10:15 Break

**Presentations by REU students (10:15AM-12:00 PM)**

10:15-10:30 **John Santiago** and Dmitry Kopelevich, "*Membrane-mediated interactions between carbon nanotubes embedded in a lipid bilayer*"

10:30-10:45 **Carolyn Worley, Alex Zakjevskii,** and Anter El Azab “*Monte Carlo simulations of SrTiO<sub>3</sub> thin film growth*”

10:45-11:00 **Brady Thompson,** “*Numerical simulations for vesicle membranes using the phase field model*”

11:00-11:15 **Shaun Pacheco** and Patrick Schelling, “*Point defects in silicate minerals studied using empirical potentials*”

11:15-11:30 **Kevin Kern,** James Kruczek, and Sagar Pandit, “*Geometric hashing: a numerical simulation of organic structures*”

11:30-11:45 **Will Molden,** Debosruti Dutta, Venkat Bhethanabotla, “*Fe-Ni Enzyme inspired sulfur tolerant catalysts*”

11:45-12:00 **Kelsie Niffenegger,** Brian Demaske, Vasily Zhakhovsky and Ivan Oleynik, “*Formation of nanostructures at metal surface exposed to femtosecond laser pulses*”

12:00-1:00 Lunch

#### **Presentations by REU students (1:00PM-4:00 PM)**

1:00-1:15 **Alan Au** and Patrick Schelling, “*Ab initio calculations of point defects in silicate minerals*”

1:15-1:30 **Thomas O’Connor** and Talat Rahman, “*The energetics of surface exchange for Ni clusters on Cu (111)*”

1:30-1:45 **Max Petulante,** Nam Le, and Lilia Woods, “*Ab-Initio Investigation into the Band Structure of Multilayer G/h-BN Systems*”

#### **Break (1:45PM-2:00PM)**

2:00-2:15 **Kimberly Schultz (REU),** Kevin McCash, and Inna Ponomareva, “*Computational exploration of THz pulses interaction with multifunctional materials*”

2:15-2:30 **Erik Weidner (REU),** Mila Adamska, Ivan Oleynik, “*Theory and modeling of asphaltenes for nanoelectronics applications*”

2:30-2:45 **Arvjnd Srikanth (REU),** Wael Al-Sawai, and Inna Ponomareva, “*Ultrafast dynamics of ferroelectric nanowires*”

## Posters

1. **Neha Nayyar**, Volodymyr Turkowski, and Talat S. Rahman, “*Antiferromagnetic-ferromagnetic transition in Fe-Rh system*”
2. **Maral Aminpour**, Duy Le, and Talat S. Rahman, “*Physisorption of 1,4-diaminobenzene molecule on an Au(111) surface*”
3. **Alamgir Kabir**, Volodymyr Turkowski, and Talat S. Rahman, “*Magnetic properties of a Fe<sub>27</sub> cluster: A DFT+U vs. DMFT analysis*”
4. **Ghazal S. Shafai**, Marisol Alcantara Ortigiza, and Talat S. Rahman, “*Structure, vibrations, and thermodynamics at the nanoscale: An ab initio study*”
5. **Iffat Nayyar**, Enrique R. Batista, S. Tretiak, A. Saxena, D. L. Smith, and Richard L. Martin, “*Self-trapping of polarons and excitons in organic materials studied by density-functional theory*”