

**FSMS 2010 Annual Meeting
Preliminary Schedule**

Monday August 2, Harris Engineering Center (HEC) Room 125

Workshop on Career Skills (10 AM – 1 PM)

- for interested graduate students and the REU students

11:00-12:00 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.

12:00-1:30 Lunch

Presentations by REU students (1:40-6:00 PM)

1:30 – 1:45 Introduction & Welcome

1:45-2:00 **J. Matthew Franklin**, Yong Nam Ahn, and Dmitry I Kopelevich (UF), “Molecular dynamics simulations of interaction between a lipid bilayer and a micelle”

2:00-2:15 **Zachary McDargh** and Patrick Schelling (UCF), “Molecular-dynamics studies of thermodiffusion in binary alloys”

2:15-2:30 **Michael Pawley** and Talat Rahman (UCF), “Accounting for Van Der Waals Interactions In Large Systems”

2:30-2:45 **Thuy-My Le** and Aravind Asthagiri (UF), “The role of Cu oxidation state on CO₂ reduction on copper oxide surfaces”

2:45-3:00 **Andrew Ross**, L. Adamska, and Ivan Oleynik (USF), “First-principles investigations of graphene-metal interfaces”

3:00-3:15 **Joshua Worch** and Sanchin Shanbhag (FSU), “A quantitative method to characterize molecular weight and long chain branching in metallocene-catalyzed polyethylene”

3:15-3:30 **Chera Rogers** and Anter El Azab (FSU), “Monte Carlo Simulation of Defect Diffusion in FCC Crystals”

3:30-3:45 **Brian J. Demaske**, V. V. Zhakhovskiy, and Ivan Oleynik (USF), “Development of EAM potentials for molecular dynamics simulations of metals at extreme conditions”

3:45–4:00 Break

4:00 -4:15 **Mark Spurgeon** and Michael Leuenberger (**UCF**), “The effect of broken carbon nanotubes on the conductance of a carbon nanotube network”

4:15-4:30 **Adam Iaizzi**, Lilia Woods, and N. Lee (**USF**), “Ab-initio study of folded armchair graphene nanoribbons”

4:30-4:45 **Advaith Rao**, D. Dutta, and V. Bhethanabotla (**USF**), “Characterizing surface segregation in Fe-Ni nanoclusters using Monte-Carlo simulations”

6:30 – 8:30 Dinner – Olive Garden

Tuesday August 3, Harris Engineering Center (HEC) Room 125

8:00-8:30 **Dr. Satyender Goel** and Artem Masunov (**UCF**) “First-principles study of transition metal diatomics and clusters for multiscale modeling of carbon nanotube growth simulation”

8:30-9:00 **Mr. Yong Nam Ahn** and Dmitry I. Kopelevich, (**UF**) “Molecular transport through flexible membranes: Role of collective degrees of freedom”

9:00-9:30 **Prof. Ke-Gang Wang (FIT)** “Crossover from Phase Coarsening to Grain Growth”

9:30-10:00 **Dr. Ivan Mikhaylov** and Artem Masunov (**UCF**) “Simulation of ultrafast photoswitching materials and theoretical predictions of their design”

10:00-10:15 Break

10:15-10:45 **Mr. Li Shu**, J. G. Park, Richard Liang, B. Wang, and Chuck Zhang, (**High Performance Materials Institute, FSU**) “Multiscale stochastic conductance model of densely-packed carbon nanotube networks: Challenges and 2D modeling”

10:45-11:15 **Dr. Alex Chernatynskiy** and Simon R. Phillpot (**UF**), “Thermal conductivity anisotropy in solids”

11-15-11:45 **Sergey Stolbov (UCF)** “First-principles approach to electrocatalysis”

11:45-12:15 **Volodymyr Turkowski** and Talat Rahman (**UCF**)

12:15-12:45 **Marisol Alcantara Ortigoza** and Talat Rahman (**UCF**)

12:45-2:00 Lunch

2:00-2:30 Graduate students put up their posters

2:30 – 3:30 Poster Session (for graduate students and other undergraduates not in REU)

3:30 – 3:45 Poster and presentation awards

3:45 – 4:15 Executive meeting on FSMS 2010 and future directions for our NSF REU site

Poster Session:

1. “Phase-field simulations of 3D microstructure evolution,” **Hui Yan** and Ke-Gang Wang (FIT)
2. “Empirical potential for laser excitation of silicon,” **Lalit Shokeen** and Patrick Schelling (UCF)
3. “Molecular dynamics simulations of the amylin oligomers for design of aggregation inhibitors,” **Workalemahu Berhanu** and Artem Masunov (UCF)
4. “Prediction of Heisenberg exchange constant for transition metal and lanthanide based organometallic systems using DFT+U,” **Shruba Gangopadhyay** and Artem Masunov (UCF)
5. “First-principles studies of the oxygen reduction reaction on Pd-Co surfaces,” **Sebastian Zuluaga** and Sergey Stolbov (UCF)
6. “TDDFT studies of collective plasmons in small bimetallic clusters,” Neha Nayyar, Alamgir Kabir, Volodymyr Turkowski, and Talat S. Rahman (UCF)
7. “Electron-Electron Correlation Effects and Magnetic Properties of Small Iron-Platinum Clusters,” **Alamgir Kabir**, Neha Nayyar, Volodymyr Turkowski and Talat S. Rahman (UCF)
8. “Effect of Ligands on the Geometric and Electronic Structure of Au₁₃ Clusters,” **Ghazal Shafaie** and Talat Rahman (UCF)
9. “Homoepitaxial Growth of Mg(0001): A First Principles Study,” **Maral Aminpour** and Talat Rahman (UCF)
10. “Inferring structural information of metallocene catalyzed polyethylenes using rheological data,” **Arsia Takeh** and Sachin Shanbhag (FSU)