

Materials for a Sustainable Energy Future

Tuesday September 17, 2013

- 2:30–3:00 **Shannon Stauffer** (University of Texas at Austin)
Characterizing States of Charge of Silicon Anodes for Lithium-ion Batteries Using an Empirical Potential
- 3:30–4:00 **Daniel Berger** (Technical University Munich (TUM))
All-electron qm/mm embedding

Thursday September 19, 2013

- 2:30–3:00 **Noa Kraitzman** (Michigan State University)
Motion of co-dimensions 1 and 2 structures under the functionalized Cahn-Hilliard Free Energy
- 3:30–4:00 **Penghao Xiao** (University of Texas at Austin)
The Challenges in Dimer Method for Saddle Point Searching

Tuesday October 1, 2013

- 2:30–3:00 **Juliana Duncan** (University of Texas at Austin)
Machine Learning Applications to Simulating Rare Events
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Ankita Katre** (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS))
Modelling Phonons in SiGe Alloys

Thursday October 3, 2013

- 2:30–3:00 **Bjoern Bieniek** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Ultra-thin ZnO Films on Metal Substrates: Suitable ZnO Surface Models or Novel Systems in Their Own Rights?
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Linas Vilčiauskas** (New York University)
DFT based molecular dynamics and proton transport: phosphates vs. water



Tuesday October 8, 2013

2:30–3:00 **Christoph Schaller** (Freie Universität Berlin)
Achieving nanometer resolution in fluorescence microscopy

Thursday October 10, 2013

2:30–3:00 **Yi Zeng** (Massachusetts Institute of Technology)
Theoretical Comparison of Dimer and Lanczos Algorithms in Minimum Mode Searching

3:30–4:00 **Anton Kollock** (Technische Universität Berlin)
An Introduction to Compressed Sensing

Tuesday October 22, 2013

2:30–3:00 **Daniel Packwood** (Tohoku University)
2D molecular magnets with weak topological invariant magnetic moments

Thursday October 24, 2013

2:30–3:00 **Nicolas Hoermann** (Universität Ulm)
Ab initio Li battery modeling

3:30–4:00 **Jakub Kaminski** (California Institute of Technology)
A new approach for the generation of heterocrystals

Tuesday October 29, 2013

2:30–3:00 **Nikhil Chandra Admal** (University of Minnesota, Twin Cities)
The interpretation of stress in molecular systems

Thursday October 31, 2013

2:30–3:00 **Maria D'Orsogna** (California State University, Northridge (CSU Northridge))
Stochastic nucleation and growth in biological systems

Tuesday November 12, 2013

- 2:30–3:00 **Mitchell Luskin** (University of Minnesota, Twin Cities)
Theory-Based Development and Benchmarking of Atomistic-to-Continuum Coupling Methods
- 3:30–4:00 **Eugene Heifets** (California Institute of Technology)
Modeling of Pathways for Oxygen Incorporation in Mixed Conducting Perovskites

Thursday November 14, 2013

- 2:30–3:00 **Gideon Simpson** (Drexel University)
Convergence Diagnostics and Discretization Effects in Parallel Replica Dynamics
- 3:30–4:00 **Nahia Mourad** (Ecole Nationale Des Ponts et Chaussees (LAMI))
On density functional perturbation theory

Monday November 25, 2013

- 11:00–12:00 **Christian Sattler** (German Aerospace Center (DLR))
Solar Cells: work carried out by the German Aerospace Center

