

## Workshop I: Quantum and Atomistic Modeling of Materials Defects

### Monday October 1, 2012

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Chris Van de Walle** (University of California, Santa Barbara (UC Santa Barbara))  
*Hybrid Functional Calculations of Defects in Materials for Optoelectronics and Quantum Information Science*
- 10:00–10:15 *Break*
- 10:15–11:05 **Peter Kratzer** (Universität Duisburg-Essen)  
*First-Principles Calculations of Point Defects in Semiconductors: Formation Energies, Electronic Properties, and Diffusion*
- 11:15–11:30 *Break*
- 11:30–12:20 **Feng Liu** (University of Utah)  
*An Efficient Method for Calculating Host and Defect Deformation Potential Based on the Concept of Quantum Electronic Stress*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Zhenyu Zhang** (University of Science and Technology of China)  
*Atomistic Formation Mechanisms and Functionalization of Epitaxial Graphene on Transition Metal Substrates*
- 3:30–4:00 *Break*
- 4:00–4:50 **Steven Valone** (Los Alamos National Laboratory)  
*Modeling Material Defects with the Fragment Hamiltonian Approach*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

### Tuesday October 2, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Arthur Voter** (Los Alamos National Laboratory)  
*Recent Developments in Accelerated Molecular Dynamics*
- 10:00–10:15 *Break*
- 10:15–11:05 **Blas Uberuaga** (Los Alamos National Laboratory)  
*Applications of Accelerated Molecular Dynamics in Materials Science*
- 11:15–11:30 *Break*

*(Tuesday schedule continued on next page)*



*(Tuesday schedule continued from previous page)*

- 11:30–12:20 **Jacques Amar** (University of Toledo)  
*Temperature-Accelerated Dynamics Simulations of Thin-Film Growth*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Tony Lelièvre** (Ecole des Ponts ParisTech)  
*Analysis of Accelerated Dynamics Methods*
- 3:00–3:15 *Break*
- 3:15–4:05 **Roger Smith** (Loughborough University)  
*Atomistic Modelling and Control of Defects Produced in Thin Film Growth*
- 4:15–4:30 *Break*
- 4:30–5:20 **Yvon Maday** (Université de Paris VII (Denis Diderot) et Université de Paris VI (Pierre et Marie Curie))  
*Finite Element Approximation for Electronic Structure Calculations*

### Wednesday October 3, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Richard Hennig** (Cornell University)  
*Control of Nanocrystal Morphology and Assembly and Quantum Monte Carlo Method for Solvation*
- 10:00–10:15 *Break*
- 10:15–11:05 **Gianfranco Pacchioni** (University of Milano-Bicocca)  
*Theory of Magnetic Impurities in Insulating and Semiconducting Oxides. Problems (and Solutions?)*
- 11:15–11:30 *Break*
- 11:30–12:20 **Nick Kioussis** (California State University, Northridge (CSU Northridge))  
*DFT Calculations of Stability and Mobility of Point Defects in Metals*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Vikram Gavini** (University of Michigan)  
*Electronic Structure Calculations at Macroscopic Scales*
- 3:00–3:15 *Break*
- 3:15–4:05 **Susan Sinnott** (University of Florida)  
*Development and Application of Charge Optimized Many-Body (COMB) Potentials to Surface Chemistry and Heterogeneous Material Interfacial Interactions*
- 4:15–4:30 *Break*
- 4:30–5:20 **Gang Lu** (California State University, Northridge (CSU Northridge))  
*Quantum Mechanics Based Multiscale Modeling of Materials*

## Thursday October 4, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung GmbH)  
*Ab initio Computation of Free Energies*
- 10:00–10:15 *Break*
- 10:15–11:05 **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Van der Waals Interactions in Molecules and Condensed Matter, including Systems with Defects*
- 11:15–11:30 *Break*
- 11:30–12:20 **Jutta Rogal** (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS))  
*Solid-Liquid Interface Free Energies and Structural Phase Transformations - Atomistic Approaches for Rare Event Systems*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))  
*Multigrid Methods in Multiscale Modeling of Atomistic Solids*
- 3:30–4:00 *Break*
- 4:00–4:50 **Lin Lin** (Lawrence Berkeley National Laboratory)  
*Towards Direct and Accurate ab initio Modeling of Material Defects at Large Scale*

## Friday October 5, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **David Ceperley** (University of Illinois at Urbana-Champaign)  
*Prospects for Quantum Monte Carlo Methods for Calculating Defects in Materials*
- 10:00–10:15 *Break*
- 10:15–11:05 **Jonathan Weare** (University of Chicago)  
*Improved Diffusion Monte Carlo*
- 11:15–11:30 *Break*
- 11:30–12:20 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)  
*The Kohn-Sham Model for Crystals with Local Defects*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Gabriel Stoltz** (École Nationale des Ponts-et-Chaussées (ENPC))  
*The Microscopic Origin of the Macroscopic Dielectric Permittivity of Crystals*
- 3:30–4:00 *Break*

*(Friday schedule continued on next page)*

*(Friday schedule continued from previous page)*

4:00–4:50     **Sidney Yip** (Massachusetts Institute of Technology)  
*Slow Dynamics: A Case Study*

