

## Materials Defects: Tutorials

Tuesday September 11, 2012

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–9:45 **Tim Schulze** (University of Tennessee)  
*Materials Defects: Tutorial and Long Program Overview*
- 9:45–10:00 *Break*
- 10:00–11:15 **Peter Voorhees** (Northwestern University)  
*DEFECTS IN CRYSTALS: DISLOCATIONS, INTERFACES AND GRAIN BOUNDARIES (Part 1)*
- 11:15–11:30 *Break*
- 11:30–12:00 *Orientation: IPAM Staff*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Danny Perez** (Los Alamos National Laboratory)  
*Introduction to Molecular Dynamics*
- 3:15–3:45 *Break*
- 3:45–5:00 **Peter Voorhees** (Northwestern University)  
*DEFECTS IN CRYSTALS: DISLOCATIONS, INTERFACES AND GRAIN BOUNDARIES (Part 2)*

Wednesday September 12, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Kristen Fichthorn** (Pennsylvania State University)  
*An Introduction to Theoretical Methods for Describing Rare Events*
- 10:15–10:45 *Break*
- 10:45–12:00 **Peter Voorhees** (Northwestern University)  
*The Thermodynamics of Crystalline Interfaces: Thermodynamics at the Nanoscale*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Danny Perez** (Los Alamos National Laboratory)  
*Introduction to Accelerated Molecular Dynamics*
- 3:15–3:45 *Break*
- 3:45–5:00 **Tony Lelièvre** (École Nationale des Ponts-et-Chaussées (ENPC))  
*Monte Carlo methods in molecular dynamics Part 1: Sampling the canonical distribution and computing free energy differences*



## Thursday September 13, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Kristen Fichthorn** (Pennsylvania State University)  
*An Introduction to Rare Event Simulation*
- 10:15–10:45 *Break*
- 10:45–12:00 **Ken Elder** (Oakland University)  
*Non-equilibrium pattern formation in materials physics*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Maria Emelianenko** (George Mason University)  
*Mathematical modeling of interfacial dynamics in polycrystals*
- 3:15–3:45 *Break*
- 3:45–5:00 **Peter Smereka** (University of Michigan)  
*Theory and Application of Simplified Kinetic Monte Carlo Models (KMC Short Course - Part 1)*

## Friday September 14, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Gabor Csányi** (University of Cambridge)  
*State of the art: a broad-brush survey of interatomic potentials (Part 1)*
- 10:15–10:45 *Break*
- 10:45–12:00 **Tony Lelièvre** (École Nationale des Ponts-et-Chaussées (ENPC))  
*Monte Carlo methods in molecular dynamics (Part 2)* *Monte Carlo methods in molecular dynamics Part 2: Sampling metastable trajectories*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Peter Smereka** (University of Michigan)  
*Theory and Application of Simplified Kinetic Monte Carlo Models (KMC Short Course - Part 2)*
- 3:15–3:45 *Break*
- 3:45–5:00 **Gabor Csányi** (University of Cambridge)  
*State of the art: a broad-brush survey of interatomic potentials (Part 2)*

