Short Course/Summer School

New algorithms for exploring structure and dynamics of interfaces

AMPEL/Quantum Matter Institute, UBC Vancouver, July 30, 2017

Room 311

Topic 1: The challenge of simulating over multiple time scales: A focus on Kinetic Monte Carlo methods (9:00am-12:00)

In spite of considerable advances in computational capacities over the last decades, there remains a considerable gap between experimentally relevant time scales and those accessible to atomistic simulations. This gap reflects the fundamentally multi scale nature of atomistic kinetics that can only be lifted partially through approximate methods that attempt to capture the most important aspect of specific phenomena. In this course, I will present the basic concepts of transition state theory, standard kinetic Monte Carlo and more recent algorithms such as the off-lattice kinetic Activation-Relaxation Technique.

Lecturer: Normand Mousseau (Université de Montreal)

Topic 2: Introduction to Accelerated Molecular Dynamics methods (1:30pm-4:30pm)

Molecular dynamics (MD) is an exceptionally powerful tool to investigate the dynamical evolution of atomistic systems. However, one of the critical limitations of MD is the rather stringent limit placed on accessible simulation timescales. This tutorial will introduce accelerated molecular dynamics (AMD) methods, a family of MD-based techniques that are designed to extend the simulation timescales for systems that evolve through rare, activated, events. The theoretical framework underpinning these methods will be discussed and targeted applications relevant to Materials Science presented. These will serve to illustrate how advanced simulation techniques can be used to simulate the evolution of materials over very long timescales, often revealing unexpected insights into the microscopic underpinnings of microstructural evolution, with accuracies approaching that of direct fully atomistic simulations.

Lecturer: Danny Perez (LANL)

Registration is free, please email alex.anees@ubc.ca