



# Bridging Time and Length Scales in Materials Science and Bio-Physics

## Workshop II: Multiscale Modeling in Condensed Matter and Material Sciences October 17 - 20, 2005

Organizing Committee: **Peter Kratzer** (Fritz-Haber-Institute), **Christian Ratsch** (UCLA) and **Dimitri Vvedensky** (Imperial College, London)

**Scientific Overview:** This workshop will focus on current problems in *materials sciences* that are pertinent to multi-scale modeling. Often, coarse-grained (continuum) models describe the macroscopic evolution of the system, while microscopic calculations (such as density-functional theory) are indispensable input to these models. Also, the microscopics can be influenced by long-range interactions; one important example is elasticity, and one needs to understand how continuum elasticity can be combined with atomistic or continuum simulation methods. It is the goal to bring together researchers with expertise in different theoretical approaches that are interested in solving multi-scale problems in materials science and condensed matter physics.

**Confirmed Speakers and Discussion Leaders:** **Jerry Bernholc** (North Carolina State Univ), **Michael Biehl** (Univ of Groningen), **Roberto Car** (Princeton Univ), **Emily Carter** (Princeton Univ), **Jim Evans** (Ames Laboratory), **Peter Kratzer** (Fritz-Haber-Institute), **Anupam Madhukar** (USC), **Horia Metiu** (UCSB), **Bo Person** (Forschungszentrum Jülich), **Christian Ratsch** (UCLA), **Karsten Reuter** (Fritz-Haber-Institute), **Robert Rudd** (Lawrence Livermore National Lab), **Peter Smereka** (Univ of Michigan), **Jerry Tersoff** (IBM), **David Tomanek** (Michigan State Univ), **Priya Vashishta** (USC), **Peter Voorhees** (Northwestern Univ), **Dimitri Vvedensky** (Imperial College), **Sidney Yip** (Massachusetts Institute of Technology)

## Mini-Workshop: Time Acceleration Methods in Atomistic Simulations October 21 - 22, 2005

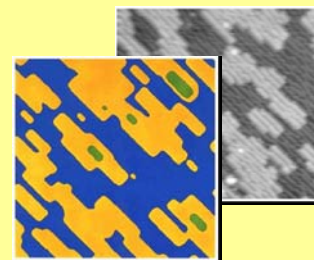
Organizing Committee: **Kristen Fichthorn** (Pennsylvania State University) and **Arthur Voter** (Los Alamos National Laboratory)

**Scientific Overview:** A significant challenge in materials sciences and biophysics is achieving long-time simulations that contain accurate atomic-scale detail. *Molecular dynamics simulations* can be based on potential energy surfaces derived from first principles and yield highly accurate dynamical information. However, these simulations cannot extend far beyond nanosecond times and often fall short of the required time scales to understand physical phenomena. In many condensed matter systems, dynamical evolution occurs via a series of rare events. A variety of methods, ranging from efficient transition state searches to kinetic Monte Carlo and accelerated molecular dynamics, have been proposed to accurately describe systems with rare-event dynamics on the mesoscale. This mini-workshop will focus on new developments in these methods and their application to problems in materials and biology.

**Confirmed Speakers and Discussion Leaders:** **Jacques G. Amar** (Univ of Toledo), **Peter Bolhuis** (Univ of Amsterdam), **David Chandler** (UC Berkeley), **Graeme Henkelman** (Univ of Texas at Austin), **Hannes Jonsson** (Univ of Iceland), **Yannis Kevrekidis** (Princeton Univ), **Alex Miron** (Fritz-Haber-Institut), **Francesco Montalenti** (Università di Milano-Bicocca), **Normand Mousseau** (Univ of Montreal), **Vijay Pande** (Stanford Univ), **Steve Stuart** (Clemson Univ), **Blas Uberuaga** (Los Alamos National Lab), **Dion Vlachos** (Univ of Delaware)

### Semester Program Schedule:

- Tutorials. September 13 - 16, 2005
- Workshop I: Multiscale Modeling in Soft Matter and Bio-Physics. September 26 - 30, 2005
- ▶ Workshop II: Multiscale Modeling in Condensed Matter and Materials Sciences. October 17 - 20, 2005
- ▶ Mini-Workshop: Time Acceleration Methods in Atomistic Simulations. October 21 - 22, 2005
- Workshop III: Density-Functional Theory Calculations for Modeling Materials and Bio-Molecular Properties and Functions – A Hands-on Computer Course. October 30 - November 5, 2005
- Workshop IV: Multiscale Analysis and Computation. November 14 - 16, 2005
- CIMMS Satellite Workshop at Caltech: Multiscale Modeling and Computation – Basic Theory and the Geosciences. November 17 - 18, 2005



**Participation:** \*\*\*The Organizers strongly encourage attendance at both workshops.\*\*\* Financial support for this workshop is available for participants at all academic levels, and recent PhD's, graduate students, and researchers in the early stages of their career are especially encouraged to apply. An online application for support is available at <http://www.ipam.ucla.edu/programs/maws2>. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission and we welcome their applications. Applicants who are interested in becoming core participants and participating in the semester program (September 12 – December 16, 2005) should apply at <http://www.ipam.ucla.edu/programs/ma2005>.

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or email questions to [maws2@ipam.ucla.edu](mailto:maws2@ipam.ucla.edu)