

FOMMS 2009 Final Program Foundations for Innovation

Sunday, July 12, 2009

6:30 – 7:30 PM **Welcoming Reception** (*Semiahmoo Ballroom Pre-function*)

7:30 – 9:30 PM **Keynote Session** (*Blakely/Cypress Ballroom*)
Presiding: Conference Chair, Sharon Glotzer, University of Michigan

7:30 Welcome Address

7:45 **Keynote Address**
The Future of Simulation Is Not What It Used To Be
Professor Daan Frenkel
Department of Chemistry, University of Cambridge

8:30 **Keynote Address**
Reverse Coarse Graining: Designing Materials that Work
Professor Berend Smit
University of California, Berkeley

9:15 Discussion

9:30 – 11:00 PM **Hospitality** (*Victoria Room*)

Monday, July 13, 2009

Monday general sessions are in the Blakely/Cypress Ballroom

8:30 – 11:50 AM Session 1: **Modeling and Simulation of Biological Systems**
Presiding: Conference Co-Chair, Susumu Okazaki, Nagoya University
 Carol Hall, North Carolina State University

8:30 *From Prediction of Structure to Design of Function*
Professor David Baker
Department of Chemistry, University of Washington

9:20 *Constant pH Molecular Dynamics*
Professor Charles Brooks
Department of Chemistry, University of Michigan

10:10 BREAK

10:30 *Molecular Understanding of Protein-surface Interactions*
Professor Shaoyi Jiang
Department of Chemical Engineering, University of Washington

11:20 Panel Discussion

2:00 – 4:30 PM **Contributed Poster Session I** (*San Juan Ballroom*)
Presiding: Conference Co-Chair Jonathan Moore, The Dow Chemical Company

7:00 – 9:10 PM Session 2: **Linking Process Scale Simulation and Molecular Simulation**
Presiding: Phil Westmoreland, NSF & North Carolina State University
 Claire Adjiman, Imperial College

7:00 *Discovery through Complex Reaction Networks*
Professor Linda Broadbelt
Department of Chemical and Molecular Engineering, Northwestern University

7:50 BREAK

8:00 *Hierarchical Multiscale Modeling and Control of Nanomaterials*
Professor Dion Vlachos
Department of Chemical Engineering, University of Delaware

8:50 Panel Discussion

9:30 – 11:00 PM **Hospitality** (*Victoria Room*)

Tuesday, July 14, 2009

Tuesday AM sessions are in the Blakely/Cypress Ballroom

8:30 – 11:50 AM **Session 3: Simulating Rare Events**
Presiding: Edward Maginn, University of Notre Dame
 Daniela Kohen, Carlton College

8:30 *Recent Advances in Path Sampling: Accurate Reaction Coordinates, Likelihood Maximization, and Diffusive Barrier Crossing Dynamics*
Professor Baron Peters
Department of Chemical Engineering, University of California, Santa Barbara

9:20 *Minimum Free Energy Path by the String Method*
Professor Giovanni Ciccotti
Department of Chemistry, University of Rome, La Sapienza

10:10 BREAK

10:30 *Taming and Exploiting Chaos in Order to Effectively Simulate Long Trajectories*
Professor Phillip Geissler
Department of Chemistry, University of California, Berkeley

11:20 Panel Discussion

7:00 – 9:30 PM **Tutorial – Molecular Simulation on Graphics Processors**
 (Blakely/Cypress Ballroom)
Presiding: Joshua Anderson, University of Michigan
 Sharon Glotzer, University of Michigan

9:30 – 11:00 PM **Hospitality** *(Victoria Room)*

Wednesday, July 15, 2009

Wednesday AM sessions are in the Blakely/Cypress Ballroom

8:30 – 11:50 AM Session 4: **Soft Materials and Complex Fluids**
Presiding: Amalie Frischknecht, Sandia National Laboratories
 Arthi Jayaraman, University of Colorado, Boulder

8:30 *Structure, Solvation, and Phase Equilibria in Hydrogen-bonding Systems*
Professor J. Ilja Siepmann
Department of Chemistry, University of Minnesota

9:20 *A Molecular Based Approach to Modeling Complex Fluids*
Professor Clare McCabe
Department of Chemical & Biomolecular Engineering, Vanderbilt University

10:10 BREAK

10:30 *Computational Studies of Capillary Phenomena: The Effects of Aerogel Compliance on Adsorptive Behavior*
Professor Lev Gelb
Department of Chemistry, Washington University, St. Louis

11:20 Panel Discussion

1:30 - 4:00 PM **Contributed Poster Session II** (*San Juan Ballroom*)
Presiding: Conference Co-Chair Jonathan Moore, The Dow Chemical Company

3:30 – 5:00 PM **Workshop on Simulation in Education** (*Victoria Room*)
Presiding: David Kofke, State University New York, Buffalo
 Andrew Schultz, State University New York, Buffalo

Wednesday PM sessions are in the San Juan Ballroom

7:00 – 9:45 PM Session 5: **Industrial Applications of Simulation-Based Engineering and Science**
Presiding: Conference Co-Chair Alain Fuchs, ParisTech
 Shiaki Hyodo, Toyota Central R&D Labs., Inc.

7:00 *Simulation Strategies Versus Experiment in Hybrid Organic-Inorganic Frameworks*
Professor Caroline Mellot-Draznieks
University College London

7:40 BREAK

7:50 *Contribution of Computational Science and Simulation in Industrial Research, Focusing on Two Recent Activities: Photonic Molecular Design and NMR Chemical Shift by FMO Method*
Dr. Shinichiro Nakamura
Mitsubishi Chemical, Japan

8:30 *Applications of DFT to a Better Understanding and Design of Industrial Catalysts in Refining and Petrochemistry*
Dr. Herve' Toulhoat
IFP, France

9:10 Panel Discussion

9:45 – 11:00 PM **Hospitality** (*Victoria Room*)

Thursday, July 16, 2009

Thursday sessions are in the San Juan Ballroom

8:30 – 11:50 AM **Session 6: Future and Emerging Computer Architectures for Molecular Simulation: Towards Petascale Simulation**
Presiding: Peter Cummings, Vanderbilt University

8:30 *Large-size, Long-time, Molecular Dynamics Simulations on a Budget*
Professor Klaus Schulten
Department of Biophysics, University of Illinois, Urbana-Champaign

9:20 *Millisecond-Long Molecular Dynamics Simulations of Proteins on the Anton Machine*
Professor David Shaw
D.E. Shaw Research and Columbia University

10:10 BREAK

10:30 *Multiscale Modeling of the Human Arterial Tree*
Professor George Karniadakis
Department of Applied Math, Brown University

11:20 AM Panel Discussion

2:00 – 3:30 PM **Workshop on Open Source Code Development**
Presiding: David Kofke, State University New York, Buffalo
 Andrew Schultz, State University New York, Buffalo
Co-Presiding: Sharon Glotzer, University of Michigan
 Peter Cummings, Vanderbilt University
 Lev Gelb, Washington University, St. Louis

5:00 – 6:15 PM **FOMMS Medal Lecture**
Professor Michele Parrinello, ETH Zurich
Presiding: Conference Co-Chairs: Sharon Glotzer and Alain Fuchs
 Introduction: Peter Cummings, Vanderbilt University

6:30 – 9:30 PM **Chairs' Reception & Conference Banquet** (*Dock and Tent*)
FOMMS: The Movie