

## Series Editor's Preface

This is the first volume in the new series *Molecular Modeling and Simulation—Application and Perspectives*. The series aims at providing a comprehensive collection of works on developments in molecular modeling and simulation, particularly as applied to the various research fields of engineering. The goal is to cover a broad range of topics related to modeling matter at the atomistic level and to provide timely and detailed treatment of advanced methods and their application in a broad range of interrelated fields such as biomedical and biochemical engineering, chemical engineering, chemistry, molecular biology, mechanical engineering, and materials science. It is therefore fitting that the first volume contains papers arising from work presented at the 2015 Foundations of Molecular Modeling and Simulation (FOMMS) conference, held July 12–16, 2015 near Mount Hood, Oregon.

I wish to acknowledge the tireless efforts of the FOMMS 2015 conference cochairs Claire S. Adjiman (Imperial College London) and David A. Kofke (University at Buffalo) and conference chair Randall Q. Snurr (Northwestern University), who organized FOMMS 2015 and carried out the editorial duties associated with assembling this volume.

Edward Maginn

# Preface

This volume contains ten papers from the 2015 conference on Foundations of Molecular Modeling and Simulation (FOMMS). The theme of this 6th FOMMS conference was Molecular Modeling and the Materials Genome. As in past conferences, the format consisted of invited lectures, contributed posters, and several workshops. A total of 172 people participated in FOMMS 2015, and 116 contributed posters were presented.

The conference began with a keynote address from Frank Stillinger of Princeton University, entitled “Chiral Symmetry Breaking via Computer Simulation.” The theme of the first session was Future Trends in Modeling, Simulation and Data Mining, and the session featured talks by Andrea Browning of Boeing, Alán Aspuru-Guzik of Harvard University, and Jinghai Li of the Chinese Academy of Sciences. The session on Biomaterials and Biological Systems consisted of talks from Sabrina Pricl of the University of Trieste and Yiannis Kaznessis of the University of Minnesota. Chris Wolverton of Northwestern University, Kristen Fichthorn of Penn State University, and Jonathan Moore of Dow Chemical spoke in the session on Energy and Environmental Applications, and the session on Complex Fluids and Materials featured talks by Edward Maginn of the University of Notre Dame, Coray Colina of Penn State University, and Marjolein Dijkstra of Utrecht University. Talks by Joachim Sauer of Humboldt University, Daniela Kohen of Carleton College, and Jeffrey Errington of the University at Buffalo were the focus of the session on Catalysis and Interfaces. The session on Reactive Force Fields featured presentations by Susan Sinnott of the University of Florida and Adri van Duin of Penn State University. The conference ended with the awarding of the FOMMS Medal to Carol Hall of North Carolina State University, who gave a memorable talk entitled “Protein Aggregation Simulations: Lessons Learned Over a Decade.”

The conference also featured three workshops. The first workshop on Data Mining, Machine Learning, and Materials Informatics was given by Jonathan Moore of Dow Chemical and Johannes Hachmann of the University at Buffalo. Joshua Anderson of the University of Michigan put on a workshop entitled “Using

GPUs for Bigger and Faster Simulations,” and the final workshop, entitled “Solving Common Software Problems in Computational Labs,” was led by Patrick Fuller of NuMat Technologies and Christopher Wilmer of the University of Pittsburgh.

The principal sponsor of FOMMS 2015 was the CACHE Corporation, with financial support coming from the Computational Molecular Science and Engineering Forum of the American Institute of Chemical Engineers, ExxonMobil, Imperial College London, the Journal of Physical Chemistry, Materials Design, the National Institute of Standards and Technology, the National Science Foundation, Northwestern University, Procter and Gamble, the Royal Society of Chemistry, Scienomics, Springer, the University of Minnesota Nanoporous Materials Genome Center, and UOP.

The ten papers in this volume represent the wide range of molecular modeling tools and applications discussed at the conference. The first paper, by Shao and Hall, presents a coarse-grained model that accounts for protein–protein interactions in a multiprotein system using discontinuous molecular dynamics simulations. The model should set the stage for simulating protein systems on longer timescales and deepening our understanding of processes such as protein crystallization, protein recognition, and protein purification. In the second paper, Sprenger et al. describe their use of molecular dynamics simulations with enhanced sampling methods to study how two types of defects in self-assembled monolayers affect the structure of adsorbed peptides. Moore et al. present the development of a coarse-grained force field for water via multistate iterative Boltzmann inversion. The model is derived to match the bulk and interfacial properties of liquid water. Hülsmann et al. discuss strategies and software for the semi- or fully-automated parameterization of force fields, including options for intramolecular and intermolecular interactions and a work flow combining global and local optimization procedures. In another paper focused on software and methods, Klein et al. describe open-source software called mBuild, which is a general tool designed to simplify the construction of complex, regular, and irregular structures for molecular simulation. Basic molecular components are connected using an equivalence operator which reduces and often removes the need for users to explicitly rotate and translate components as they assemble complex systems. In a methods-oriented contribution bridging quantum and classical mechanics, Subramanian et al. examine the Path Integral Monte Carlo performed with “semi-classical beads.” They compare the rate of convergence with respect to the number and type of beads for computing fully quantum virial coefficients of helium-4.

Turning more toward applications, the paper by He et al. describes molecular simulations of the homogeneous nucleation of the ionic liquid  $[\text{dmim}^+][\text{Cl}^-]$  from its bulk supercooled liquid. Their work combines the string method in collective variables, Markovian milestoneing with Voronoi tessellations, and order parameters for molecular crystals. Results include the free-energy barrier, the critical nucleus size, and the nucleation rate. Schweizer et al. study the influence of alloy composition on the structure of Raney nickel catalysts using molecular dynamics simulations and the competitive adsorption of benzene and cyclohexane on Raney nickel as a first step toward modeling the catalytic hydrogenation of benzene. Norman

et al. present atomistic modeling related to hydrocarbon mixtures and gas hydrates in porous media, including molecular dynamics simulations to study the phase diagrams of hydrocarbon mixtures in the bulk and in confined geometries. Finally, Bamberger and Kohen report a combination of grand canonical Monte Carlo and MD simulations that provide new insight into an intriguing “cation gating” that allows carbon dioxide but not other adsorbates to permeate Na—Rho zeolites.

We thank all of the participants for their contributions to FOMMS 2015 and especially the authors and reviewers of the papers in this volume. Special thanks goes to the conference facilitator, Robin Craven; the Senior Advisors of FOMMS 2015, Peter Cummings, Joe Golab, Clare McCabe, Jonathan Moore, and J. Ilja Siepmann; and the conference Programming Committee.

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