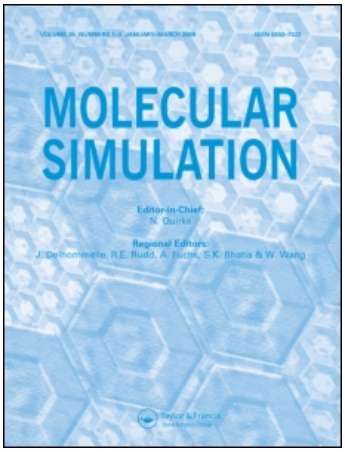

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Guest Editorial: Frontiers of Molecular Simulation

J. Delhommelle[a]
[a] Department of Chemical Engineering, University of South Carolina, Columbia, SC, USA

To cite this Article Delhommelle, J.(2006) 'Guest Editorial: Frontiers of Molecular Simulation', Molecular Simulation, 32: 3, 173 — 174
To link to this Article: DOI: 10.1080/08927020600686845
URL: http://dx.doi.org/10.1080/08927020600686845

Molecular Simulation, Vol. 32, Nos. 3–4, 15 March–April 2006, 173–174

Taylor & Francis
Taylor & Francis Group

Guest Editorial: Frontiers of Molecular Simulation

The 2005 American Institute for Chemical Engineers (AIChE) Annual Meeting was held in Cincinnati, OH, October 30–November 4, 2005. This special issue of Molecular Simulation is a selection of fifteen papers presented during the Computational Molecular Science and Engineering Forum.

The Computational Molecular Science and Engineering Forum consisted of twenty-four sessions. One third of the sessions were devoted to the improvements of simulation models and methods (developments in intermolecular potential models, recent advances in molecular simulation methods and more particularly in hybrid multiscale simulations). The first three papers of this special issue are selected from these sessions. Jianguo Dai *et al.* present a lattice kinetic Monte-Carlo model for vacancy diffusion and aggregation in crystalline silicon at elevated temperatures. Jayeeta Ghosh *et al.* apply two recent developments in molecular simulation methods, the density of states (Wang-Landau) Monte-Carlo method and a multiscale modeling method, to improve our understanding of the glass transition. Richard Sadus shows how simulations can be used to understand a wide variety of phenomena ranging from the role played by three-body interactions in phase equilibria to the differences in transport properties between dendrimers and conventional polymers.

In recent years, the study of biological systems has become a significant part of the research carried out in the field of Chemical Engineering. This annual meeting was a reflection of this evolution since five sessions addressed the topical issues of computational biology and computational genomics. Six papers selected in this issue describe how simulation can shed light on such systems. Mike King, Chair of the sessions on Computational Biology, comments on the most active areas of research in the field (simulation and prediction of gene network, simulations—either fully atomistic or coarse-grained—of lipid membranes and membrane/protein interactions and multiscale simulations of receptor-mediated blood cell adhesion under flow). Allison Langham *et al.* study the effects of mutations at the C-terminus of Protegrin-1 and used their observation to rationalize the design of novel peptide sequences that are antimicrobial but not toxic. Patrick Walton, Chair of the sessions on Computational Genomics, *et al.* explain how recent contributions to the computational analysis of high-throughput, multi-source data have made a considerable impact towards the computational elucidation and analysis of cellular pathways and networks. Jhih-Wei Chu *et al.* present two new approaches for obtaining coarse-grained force fields from atomistic molecular dynamics trajectory and demonstrated the performance of their methods on a study of a DMPC lipid bilayer and of the mechanical behavior of actin filaments. Sukit Leekumjorn *et al.* study the interactions of trehalose with lipid bilayers of DPPC, DPPE and their mixture. Sandeep Patel *et al.* describe their recent advances in the development of fluctuating charge force fields as well as recent applications to a spectrum of chemical and biological systems such as small molecule liquid–vapor interfaces, solvated proteins/peptides and physiological membrane systems.

The third part of this special issue consists of six papers presenting industrial applications of molecular simulations. The first two papers deal with alternative sources of energy, i.e. fuel cells and hydrogen storage materials. Bill Goddard *et al.* described how they developed a reactive force field, based first principle quantum mechanics, and how this force field can be used to develop a predictive model to estimate the changes in performance of fuel cells systems upon changes in design. Dubravko Sabo *et al.* investigated the stability of hydrogen clathrate hydrates under ambient conditions and the ability of those systems to serve as a means to efficiently store molecular hydrogen. The next two papers are examples of Computer Aided Molecular Design (CAMD). Ioana Stanescu *et al.* use CAMD to design candidate solvents for the Kolbe-Schmitt reaction and carry out *ab initio* calculations to test the ability of those

Molecular Simulation
ISSN 0892-7022 print/ISSN 1029-0435 online © 2006 Taylor & Francis
http://www.tandf.co.uk/journals
DOI: 10.1080/08927020600686845

solvents to improve the reaction rate of the Kolbe-Schmitt reaction. Sarah Thompson *et al.* propose to apply CAMD to design polymers with the ability to stabilize a model peptide drug. In the next paper, Gustavo Caballero *et al.* investigate the effect of the nanocluster size on surface segregation phenomena of Pt/Pd alloys and look into the implications of their findings on catalytic processes. In the last paper of this special issue, Saadet Ulas *et al.* apply sampling techniques based on quasi-random numbers to the calculation of solvent-water partition coefficients with the aim of design more environmentally benign processes.

We would like to express our appreciation to the reviewers for their strong comments. We would also like to thank Nick Quirke, Editor-in-Chief of Molecular Simulation and Michelle Burns, Production Editor, for helping us prepare this special issue.

J. Delhommelle
Department of Chemical Engineering
University of South Carolina
310 Main Street South
Columbia, SC 29201 USA