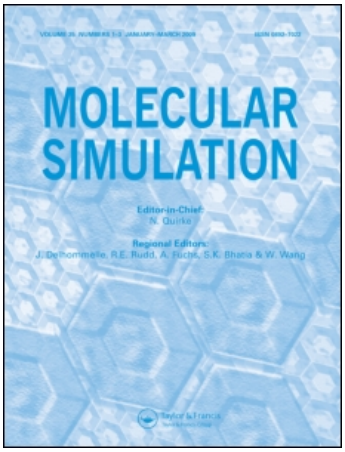

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Recent developments in molecular simulation

Jerome Delhommelle[a]
[a] University of North Dakota,

Online publication date: 03 August 2010

To cite this Article Delhommelle, Jerome(2010) 'Recent developments in molecular simulation', Molecular Simulation, 36: 7, 497
To link to this Article: DOI: 10.1080/08927022.2010.504409
URL: http://dx.doi.org/10.1080/08927022.2010.504409

Molecular Simulation
Vol. 36, Nos. 7–8, June–July 2010, 497

GUEST EDITORIAL

Recent developments in molecular simulation

This special issue is a selection of 14 papers reflecting the recent developments in the field of molecular simulation in the chemistry and chemical engineering community. As it has been the tradition for the past four special issues on this topic, most of these papers were presented during the 2009 AIChE (American Institute for Chemical Engineers) Annual Meeting in Nashville, TN. The applications and topics discussed in this issue can be divided into four categories: (i) new molecular simulation methods, with an emphasis on the determination of free energies, (ii) applications to the determination of phase behaviour, (iii) simulation studies of transport in molecular and biological systems, and (iv) classical or density functional theory studies of heterogeneous systems, with a focus on catalysis.

The first part of this special issue is devoted to the development and applications of new molecular simulation methods. Nathan Duff and Baron Peters propose a mitosis method to calculate directly the interfacial free energy of nuclei in solution. Scott Shell presents a methodology, based on replica-exchange molecular dynamics simulations, to compute the relative free energies of peptide conformational states. Gerassimos Orkoulas details how spatial updating can be applied to Monte Carlo simulations of atomic systems. Filip Moučka and Ivo Nezbeda discuss technical as well as physical aspects of the multi-particle move Monte Carlo scheme.

The second part of this special issue focuses on simulations, which aims to accurately predict the phase behaviour of fluids. Daniel Noon and Gerassimos Orkoulas discuss the simulation of phase transitions via spatial updating and tempering. Caroline Desgranges et al. detail how multiple time step hybrid Monte Carlo Wang–Landau simulations in the isobaric–isothermal ensemble may be optimised to determine the phase equilibria of branched alkanes.

The third part of the issue deals with simulation studies of transport in molecular and biological systems. Nikolaos Voulgarakis et al. present simulation methodologies to model the viscoelasticity and thermal fluctuations of fluids at the nanoscale. Yanmei Song and Lenore L. Dai discuss simulation results on the shear viscosities of common water models by non-equilibrium simulation methods. Esai Selvan et al. discuss how reactive molecular dynamics can be applied to study proton transport in systems of water confined in carbon nanotubes. Ateeque Malani et al. present molecular dynamics simulation results on the hydration of ions under confinement.

The last part of the special issue is devoted to applications of classical molecular dynamics simulations or density functional theory studies of heterogeneous systems, with a focus on catalysis. Rebecca Cantrell and Paulette Clancy use molecular dynamics simulation to study the effect of pentacene polymorphs on C_{60} surface adsorption and diffusional properties, and on the tendency to form nanowires. Beverly Hinojosa et al. discuss density functional theory results on the adsorption and dissociation of water on the $SrTiO_3$ (100) surface. Run Long and Niall English present density functional theories of doping in titania. Nilay İnoğlu and John Kitchin present a tight-binding model parametrised by a database of density functional theory calculations to estimate the d-band characteristics of bulk as well as mono- and bimetallic surface structures.

We would like to express our appreciation to the reviewers for their invaluable contribution. We would also like to thank Nick Quirke, Editor-in-Chief of *Molecular Simulation*, and Ryan Kidd for helping us prepare this special issue.

Jerome Delhommelle
University of North Dakota
Email: jdelhommelle@chem.und.edu

ISSN 0892-7022 print/ISSN 1029-0435 online

DOI: 10.1080/08927022.2010.504409
http://www.informaworld.com