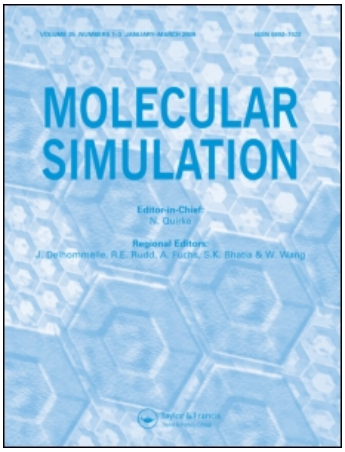

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Guest editorial: Recent developments in molecular simulation

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Guest editorial: Recent developments in molecular simulation

The 2006 American Institute for Chemical Engineers (AIChE) Annual Meeting was held in San Francisco, CA, November 12–17, 2006. This special issue of *Molecular Simulation* is a selection of sixteen papers presented during the thirty-one sessions of the Computational Molecular Science and Engineering Forum.

The first part of this issue is devoted to recent advances in molecular simulation methods, multiscale modelling and to developments in intermolecular potential models. Cristopher P. Calderon and Ioannis G. Kevrekidis develop an efficient estimation strategy, which uses the output of short bursts of atomistic simulation, to enhance fine scale simulations of chemically reacting systems. Jianguo Dai *et al.* present a lattice kinetic Monte Carlo model for vacancy aggregation to investigate the morphological evolution of large vacancy aggregates under different conditions relevant to commercial silicon crystal growth. Hendrik Heinz proposes a simple method to calculate local and average pressure tensors in simulations of molecular systems. Jayeeta Ghosh and Roland Faller apply systematic structural coarse-graining based on optimizing a potential against the structure obtained in atomistic simulations to a small organic glass former ortho-terphenyl (OTP). MaryBeth H. Ketko and Jeffrey J. Potoff study the effect of partial charge parametrization on the fluid phase behavior of dimethyl ether (DME) using grand canonical Monte Carlo simulations combined with histogram reweighting techniques. Using Monte Carlo reweighting techniques with either a fourth order cumulant calculation or a mixed field study, Javier Perez-Pellitero *et al.* determine the critical points and the vapor liquid equilibria of thiophene, 2-methylthiophene and 2,5-dimethylthiophene modeled with the Anisotropic United Atoms model AUA4.

The second part of this special issue consists of three papers presenting applications of molecular simulations to model biological systems. E. R. May *et al.* use coarse-grained molecular dynamics simulations to understand the effect of the addition of phosphatidyl-inositol-4-phosphate lipids on the elastic properties of dipalmitoyl phosphatidyl choline (DPPC) lipid bilayers. S. K. Kandasamy and R. G. Larson apply molecular dynamics simulations to study the interaction between a beta-strand antimicrobial peptide, protegrin-1, and model lipid bilayers of different hydrophobic widths. D. Bolintineanu *et al.* carry out molecular dynamics simulations of the naturally-occurring protegrin PG-1 peptide and two of its mutants, PC-9 and PC-13, in the presence of a dodecyl-phosphocholine (DPC) micelle.

We gather in the third part of this issue three contributions dealing with adsorption phenomena. D. D. Do and H. D. Do propose to use defected walls of carbon pores to model adsorption and apply their approach to derive the pore size distribution of Saran charcoals from experimental data on argon and nitrogen adsorptions. J.-M. Simon *et al.* apply nonequilibrium molecular dynamics simulations to provide numerical evidence of a thermal driving force during the adsorption of butane in silicalite. R. R. Kotdawala *et al.* use Monte Carlo simulations to understand and characterize the adsorption of hydrogen cyanide and methyl ethyl ketone in silicalite-1, mordenite and zeolite beta structures.

The fourth part of this special issue consists of four papers presenting industrial applications of molecular simulations. Ioannis Economou *et al.* use molecular simulation and macroscopic (equation of state) modeling to evaluate the solubility of *n*-alkanes, perfluoroalkanes noble and light gases in four elastomer polymers. Yao Houndonougbo *et al.* review their recent work on the calculations of the phase equilibrium and transport properties in carbon-dioxide expanded liquids using Gibbs Ensemble Monte Carlo and molecular dynamics simulations. Bangwu Jiang *et al.* report on nonequilibrium molecular dynamics simulations and experimental results on the rheological properties of four short-chain perfluoropolyethers. Using *ab initio* calculations, Veronique van Speybroeck *et al.* study the

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elementary reactions taking place during coke formation in a thermal cracking unit.

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 Tom Morris, Production Editor, for helping us prepare this special issue.

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