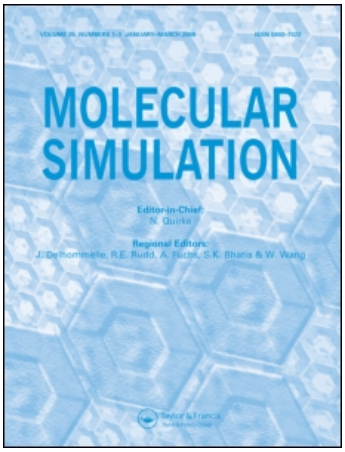

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Recent advances in molecular simulation

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GUEST EDITORIAL

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The 2007 AIChE (American Institute for Chemical Engineers) Annual Meeting was held in Salt Lake City, Utah, from 3 November to 9 November 2007. This special issue of *Molecular Simulation* is a selection of ten papers presented during the meeting.

The first part of this issue is devoted to new developments in molecular simulation methods. C. Heath Turner et al. review recent advances and applications of the Reaction Ensemble Monte Carlo method (RxMC), which aims at understanding and predicting the equilibrium behaviour of chemically reacting systems. S. Ucyigitler et al. combine Discontinuous Molecular Dynamics methods with Thermodynamic Perturbation Theory to infer transferable intermolecular potential functions. C.-Y. Chen et al. analyse phonon interactions to understand the effect of adsorbed guest molecules on the thermal conductivity of zeolites.

We gather in the second part of this issue three contributions dealing with applications of molecular simulations to model biological systems. Hongmei Liu et al. carry out molecular dynamics simulations to study the selectivity mechanism of nanopores by studying ion permeation events through non-charged carbon nanotubes. C. Desgranges et al. develop a nonequilibrium molecular dynamics simulation method, based on the transient-time correlation function formalism, to estimate the conductivity of nanoconfined liquids subjected to experimentally accessible fields. Xianghong Qian uses *ab initio* calculations to analyse the cooperative effect on hydrogen bonding interactions in native cellulose Iβ.

The third part of this special issue consists of four papers presenting industrial applications of molecular simulations. K. Hemelsoet et al. report on Density Functional Theory results of the elementary steps leading to coke growth within a steam cracking unit. G.K.P. Dathara et al. carry out Density Functional Theory calculations to investigate the structure and stability of pristine and Ti-doped $NaAlH_4$. C. Nieto-Draghi et al. optimise the dynamical behaviour of the anisotropic united atom model for branched alkanes, olefins and a model fluid gasoline. Using nonequilibrium molecular dynamics simulations, Bangwu Jiang et al. analyse and compare the rheological properties of perfluoropolyethers to that of *n*-alkanes.

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

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