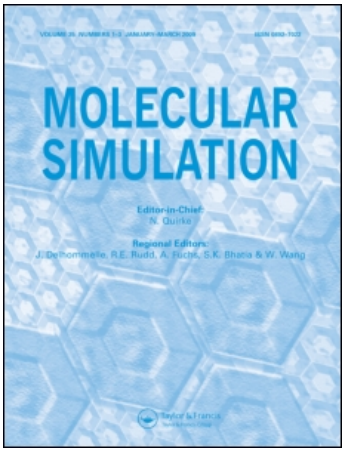

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Guest Editorial

This special issue is a selection of 21 papers presented during the 2008 American Institute for Chemical Engineers (AIChE) Annual Meeting in Philadelphia, PA. The applications and topics discussed in this issue can be divided in four categories: (i) molecular simulations of nanoparticles and other nano-sized systems, (ii) determination of free energies and phase behaviour, (iii) classical or density-functional theory studies of heterogeneous systems and (iv) coarse-grained methods and their applications to biological systems.

The first part of this special issue is devoted to the applications of molecular simulation to understand the properties of nanoparticles. Using molecular dynamics simulations, Mingxiang Luo et al. study the self-assembly of systems of surfactants and hydrocarbon nanoparticles at liquid–liquid interfaces. Julibeth Martinez De La Hoz et al. investigate the phase stability of Cu–Ag nanoalloys using the classical molecular dynamics simulations. Brian Morrow and Alberto Striolo use molecular dynamics simulations to develop an understanding of the catalytic activity of supported platinum nanoparticles. Brian Henz et al. carry out molecular dynamics simulations to develop an understanding of the kinetic sintering of Al and Ni nanoparticles. Using nonequilibrium molecular dynamics, Xiongce Zhao investigates the feasibility of a nanoscale Paul, or radiofrequency, trap for ions. Francisco Hung and Shivkumar Bale study faceted nanoparticles, immersed in a nematic liquid crystal, and determine the defect structures as well as the potentials of mean force. Arthi Jayaraman and Kenneth Schweizer develop a liquid state theory to predict the structure and the phase diagram of polymer-tethered nanoparticles. Milton Cole et al. review the application of a nanoscale Lifshitz theory, the coupled dipole method, to determine Van der Waals interactions on the nanoscale. Sangheon Lee et al. combine the Monte Carlo method with tight binding molecular dynamics and the density-functional theory to determine the structure and stability of native defects in crystalline silicon.

The second part of this special issue describes simulations, the aim of which is to accurately predict the phase behaviour as well as the free energy of fluids, mixtures and solids. Jayant Singh uses the grand-canonical transition matrix Monte Carlo simulations with the histogram reweighting technique to determine the vapour–liquid equilibria and the surface tension of hard-core Yukawa fluids. Using osmotic Gibbs Ensemble Monte Carlo simulations, Kim Bolton et al. investigate the water clustering in hydrocarbons (alkanes and polyethylene) and study the role played by the external electric fields and ionic impurities. Martin Sweatman reviews the application of the self-referential method to compute the free energy of the crystalline phases and discusses how the results of these calculations may be used to determine the solid–fluid coexistence from the adapted Gibbs ensemble Monte Carlo simulations.

The third part of the issue deals with simulations on heterogeneous systems. The methods used in this section are either purely classical, such as, for example, the determination of adsorption isotherms, or first principles molecular dynamics simulations, based on the density-functional theory, for the study, e.g., of nanocatalysts. Using the Grand Canonical Monte Carlo simulations, Ruichang Xiong et al. compute adsorption isotherms of explosives, such as RDX, in metal-organic frameworks for potential applications in the detection of explosives. Using two-dimensional cluster expansions, Spencer Miller and John Kitchin extend density-functional theory results to a wide range of configurations and calculate oxygen adsorption energies on Au and Pt (111) surfaces. Bin Liu et al. apply density-functional theory calculations to study the decomposition of hydrogen and methane on nickel nanoparticles as well as on nickel surfaces. Nilay İnoğlu and John Kitchin also use the density-functional theory methods to study sulphur poisoning on copper surfaces. Liqun Zhang et al. carry out density-functional theory calculations to determine the diffusivity of noble gases in silica melts.

The last part of the special issue is devoted to applications of coarse-grained simulation methods, with a special emphasis on biological systems. Huajun Yuan et al. develop a protocol to understand molecular transport through biological membranes and carry out coarse-grained molecular dynamics simulations using dipalmitoylphosphatidylcholine as the bilayer membrane. Jong Hyuk Pak and Andreas Heyden present a mixed-resolution simulation technique by combining an atomistic description for a small active zone with a coarse-grained model for the larger inactive zone. Using coarse-grained

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methods, Xiaoyu Wu and Ganesan Narsimhan determine the tertiary structure of lysozyme, when adsorbed on a silica surface. Abdallah Sayyed-Ahmad et al. compute the relative free energy of binding of antimicrobial peptide–micelle systems using a molecular mechanics Poisson–Boltzmann surface area protocol.

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 William Padgett, Production Editor, for helping us prepare this special issue.

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