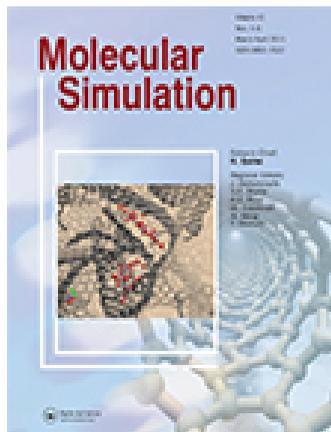


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### Guest Editorial

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## CONFINED FLUIDS

### Guest Editorial

Fluids in confined environment are increasingly playing important roles in new technologies. Hence, understanding the nature of nano-confined fluids is of direct relevance in various applications. This special issue is composed of 14 papers reflecting advances in the molecular simulation of confined fluids.

The first part of the issue is devoted to review articles. Eslami and co-workers provide a comprehensive review of simulation methods used for investigating the structure and dynamics of nano-confined fluids. While the article is focused on polymers, the methods based on molecular dynamics can also be used for non-polymeric fluids. The authors have also described the thermal properties of the confined polymers, such as thermal conductivity and the Kaptiza length, using non-equilibrium molecular dynamics. Das, on the other hand, provides a comprehensive review of the thermodynamics and kinetics of liquid–liquid coexistence under confinement using molecular simulation. The author describes the use of Monte Carlo and molecular dynamics methods to obtain the contact angle and phase coexistence information. Furthermore, kinetics of phase separation of confined fluids is also discussed by Das.

The second part of the issue focuses on the adsorption of gas and liquid molecules in confined geometries. Sengupta and Adhikari demonstrated the use of the triangle-well potential to model confined simple fluids. The contribution from my group, at the Indian Institute of Technology Kanpur, addresses the adsorption behaviour of methane and ethane in inorganic nanopores (Sharma et al.). This is important due to the need to find alternative sources of energy, and shale gas is an important candidate among many other choices. The article, in particular, presents the structural and dynamical properties of methane and ethane in montmorillonite pores. Varanasi and Yashonath studied the structural and dynamical properties of an equimolar mixture of cumene and pseudo-cumene in zeolite. The result is extremely useful, as it clearly suggests to exploit the rotational diffusivity, which is substantially different for the two molecules, in separating the two isomers. The contribution from Farmahini and Bhatia presents a realistic model of nanoporous silicon carbide-derived carbon using the hybrid reverse Monte Carlo method, and the authors demonstrate it for the

adsorption of large molecules such as propene, neopentane and sulphur hexafluoride, besides water. The authors, using grand-canonical Monte Carlo simulation and molecular dynamics, studied the diffusion and activation energy barrier of the above molecules, and also compared it with water. The adsorption behaviour of water is found to be anomalous compared with that of non-polar gases. As a limited case of confinement, Phadungbut and co-workers, who have studied adsorption of a simple fluid on a surface, report the behaviour of an argon monolayer on a graphitic surface at a temperature lower than the two-dimensional critical temperature.

The third part of the issue focuses on the confined liquid behaviour. Dos Santos and Cordeiro have studied the effect of anion replacement on the structural behaviour of an ionic liquid confined within gold channel. Kayal and Chandra explored the structure and dynamics of nano-confined water molecules using molecular dynamics simulations. Indra and Biswas have presented a work of water and surfactant systems, where, based on various properties including hydrogen bond, the water molecules tend to behave like a confined fluid. Renou and co-workers discuss the dielectric anisotropy of water confined into the metal–organic framework and carbon nanotube (CNT) using molecular dynamics. This is an important contribution considering the lack of information on the water dielectric properties of confined fluids. The authors provide a molecular interpretation of the anisotropy of the dielectric permittivity. In particular, the authors have shown that there is a dielectric anisotropy in confined fluids, which are remarkably different from the bulk properties. Singha Deb and co-workers studied the adsorption of lanthanide (III) and actinide (III), using the density functional theory, to understand the separation of the above metal ions. The authors report the free energy of complexation of lanthanide (III) and actinide (III) with functionalised CNT, which they also verified by experiments.

In the last part of the issue, transport behaviour of water in confined geometry is discussed. Kumar and co-workers raised an important question about the driving force of water entry in hydrophobic channels of CNTs. Is it entropic or energetic? On the other hand, Cheng and co-workers provide a novel device based on double-walled

carbon nanotube (DWCNT) for controllable pumping of water. The authors demonstrate, using molecular dynamics, that the uncapped DWCNT can be utilised for giant and unidirectional flow of water.

I would like to express my appreciation to the reviewers, for their invaluable contribution. I would also like to thank Nick Quirke, Editor-in-Chief of *Molecular Simulation*, Huw Price, Managing Editor, and Marina

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