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A MEAN-FIELD VIEW OF THE SCREENING EFFECT IN SIMULATIONS

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SCAN &RSVP

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ABSTRACT OF THE TALK

One of the most significant properties of ordinary condensed phase matter is the screening of Coulomb force: a system in thermal equilibrium does not tolerate any charge inhomogeneity over the range of a few intermolecular distances. As a consequence, charge distribution and correlations are subject to specific constraints. It is, however, nontrivial to develop proper handlings of the long-ranged Coulomb potential to satisfy the constraints in typical molecular dynamics and Monte Carlo simulations of explicit molecules in bulk and/or at interfaces with a finite setup of the simulation cell.

In this talk, I will suggest a symmetry-preserving mean-field (SPMF) approach, which could be extended naturally from some of the early mean-field concepts, like the seminal Debye-Huckel theory, to recover the screening condition for finite degrees of freedom. SPMF argues that certain slowly varying component of the electrostatic potential, can be replaced by its average over the degrees of freedom in the directions with preserved symmetry. In addition to provide an efficient and accurate handling of the electrostatics in molecular simulations, the involved mean-field theory predicts analytically some of the failure of the existing treatments for both bulk and interfaces, which could be verified by numerical simulations and will be the main focus of my talk.

BIOGRAPHY

Zhonghan Hu obtained his bachelor degree in chemical physics at the University of Science and Technology of China (USTC) in 2003 and his PhD degree in Chemistry with Claudio Margulis at the University of Iowa in 2007. After working as a postdoc with John Weeks at the University of Maryland, college Park and with Bruce Berne at Colombia University, he started his own group at Jilin University in August, 2010 and then moved to Shandong University at Qingdao in December, 2019. In the past, he carried out simulations of room-temperature ionic liquids to understand their transport and optical properties, and applied stochastic models to analyze biological force rupture experiments. His main research interest in the recent ten years is to understand statistical mechanics of liquids and to develop efficient techniques for handlings of electrostatics in simulations.