

Lattice models of ionic liquids in conducting slit nanoconfinement

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Confined ionic liquids exhibiting exciting physics are essential in modern technologies. The narrow conducting confinements cause exponential screening of the electrostatic interactions between ions, allowing the development of models with short-range interactions that can provide analytical insights into the charge storage mechanisms. In this contribution, we present a lattice model for ionic liquids confined in ultranarrow slit-shaped pores admitting a single layer of ions. In the case of next-nearest interactions, it can be mapped onto the well-known three-state Blume-Capel model, which obeys an analytical solution within the Bethe-lattice approximation [1]. Analyzing phase behavior and pore charging in terms of pore ionophilicity, interionic interactions, and applied potential difference, we obtained a phase diagram comprising the lines of first- and second-order, direct and re-entrant phase transitions, manifested by singularities in the capacitance-voltage dependence [2]. These analytical results are corroborated by lattice Monte Carlo simulations [3]. However, it is known that, at least in the quasi-one-dimensional case of single-file pores, the results of the lattice model with short-range interactions differ even qualitatively from the exact results of the corresponding continuous model [4]. We will discuss possible ways to improve the lattice model by considering further interactions and analyzing changes in the phase diagram depending on the interaction parameters.

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Primary author: DUDKA, Maxym

Presenter: DUDKA, Maxym

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