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Theory of electrolyte solutions in a slit charged pore: Effects of structural interactions and specific adsorption of ions

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The study of electrolyte solutions in confined geometries is crucial for developing energy storage devices and water purification systems. One challenge in this field is accurate modeling ion behavior while considering the interplay between ion-specific effects and electrostatic interactions. Although self-consistent field theory enables the simulation of ionic fluids, it overlooks several effects, such as short-range correlations of the ions. Recent research [1] incorporates into the grand thermodynamic potential of ionic fluid the short-range correlations of the ions and derives the mechanical equilibrium condition using the Noether's theorem formalism. In particular, the authors have derived the total stress tensor of ionic fluid taking into account electrostatic and steric interactions alongside the structural effects (short-range correlations).

In this work, we use the model developed by Blossey et al. [2], which takes into account both structural and steric interactions between ions. The structural interactions are described through a bilinear form of the gradients of the local ionic concentrations, while the steric interactions are modeled using the lattice gas approach.This framework allows for a phenomenological description of the molecular properties of ions, such as steric interactions due to their non-spherical shape, changes in configuration, and the influence of the solvent. Additionally, we investigate the specific interactions between ions and pore surfaces by incorporating external attractive forces.

Our main interest lies in analyzing how ionic concentration profiles and disjoining pressure are influenced by variations in pore size. Starting from the local mechanical equilibrium condition, we derive a general formula for the disjoining pressure.
Our findings [3] indicate that taking into account the structural interactions between ions leads to a pronounce minimum in the disjoining pressure curves at small pore widths. This minimum is attributed to the formation of electrical double layers on the electrically charged surfaces of the pores.In addition, our results indicate that the attractive interactions between ions and the pore walls contribute to the formation of this minimum and shift it to smaller pore sizes. These theoretical findings have practical implications for researchers in the field of electrochemical engineering for supercapacitors, particularly in applications involving porous electrodes filled with concentrated electrolytes and room temperature ionic liquids.

[1] Brandyshev P. E., Budkov Y. A. Noether's second theorem and covariant field theory of mechanical stresses in inhomogeneous ionic liquids. The Journal of chemical physics. –2023.–T. 158. –No. 17.
[2] Blossey R., Maggs A. C., Podgornik R.Structural interactions in ionic liquids linked to higher-order Poisson-Boltzmann equations. Physical Review E. –2017
[3] Victoria A. Vasileva, Daria A. Mazur, Yury A. Budkov. Theory of electrolyte solutions in a slit charged pore: Effects of structural interactions and specific adsorption of ions. Journal of Chemical Physics. 2023. Vol. 159. No. 2. Article 024709

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