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Electrosorption-induced deformation of microporous carbons: molecular dynamics and mean-field theory

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Nanoporous carbons play an important role in different electrochemical applications and, in particular, are widely used as porous electrodes in super-capacitors. Ions in aqueous electrolytes form the electrical double layer on the charged electrode-solution boundary, which can lead to a complex physical picture in nano-sized pores. In this work, using molecular dynamic simulations and the framework of the modified Poisson-Boltzmann equation [1], we studied the structure of the electrical double layer and the developed solvation pressure in slit graphitic micropores immersed into a 1:1 aqueous electrolyte. Namely, we used NaCl aqueous solution, as one of the most common. We focused on the behavior of solvation pressure as a function of pore width and surface charge density. Two different water models were used: explicit one –based on SPC/E [2] water molecule and implicit one, i.e. structureless background with fixed dielectric permittivity. The latter allows us to perform the most accurate comparison between molecular dynamics and theory. We demonstrated that the theory could predict the solvation pressure dependence on the pore width almost quantitatively correctly compared with the results using the implicit water model. In turn, the simulations with explicit water show the qualitatively different behavior of the solvation pressure in 1 nm and 2 nm pores as a function of surface charge density. We demonstrated that the value of the solvation pressure is defined by a delicate balance between Van der Waals and electrostatic contributions. Finally, using the theoretical approach we estimated the solvation pressure on the macroscopic scale using earlier developed approach [3], which have been developed to describe adsorption-induced deformation. Our results can be used in the further development of a theoretical framework for the description of electrosorption-induced deformation.

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References

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