

Negative Pressure of Ionic Liquids Inside a Nanoslit: Molecular Dynamics Study

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Recently, our group has been focused on the osmotic pressure of an electrolyte in a nanoconfinement. It is directly related to the stress acting on the electrode wall, which can induce deformation of porous electrodes. Generally, the electrolyte inside the nanoconfinement would exert a pushing (outward) force on the wall, but when the nanoslit width became comparable to the ion size, the pulling (inward) force was observed contrary to popular belief. Since it is a trend to reduce the size of the nanopore for the efficiency of the electric system, it is very important to understand this antipode for the system stability. This inward (negative) nature of the pressure was a result of a competition between the Maxwell stress and contact contributions of internal electrolyte. In this work, we investigated the negative pressure in a charged nanoslit with different combinations of ionic liquid electrolyte. The scale of negative pressure acting on the nanoslit wall and effects of ion size and shape on the pressure are analyzed with the ion layer structure.