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Prediction of Osmotic Pressure of Ionic Liquids Inside a Nanoslit by MD Simulation and Continuum Approach[1] GI JONG MOON, YU DONG YANG, Department of Chemical Engineering, POSTECH, JUNG MIN OH, Center for Soft and Living Matter, Institute for Basic Science (IBS), IN SEOK KANG, Department of Chemical Engineering, POSTECH — Osmotic pressure plays an important role in the processes of charging and discharging of lithium batteries. In this work, osmotic pressure of the ionic liquids confined inside a nanoslit is calculated by using both MD simulation and continuum approach. In the case of MD simulation, an ionic liquid is modeled as singly charged spheres with a short-ranged repulsive Lennard-Jones potential. The radii of the spheres are 0.5nm, reflecting the symmetry of ion sizes for simplicity. The simulation box size is 11nm11nm7.5nm with 1050 ion pairs. The concentration of ionic liquid is about 1.922mol/L, and the total charge on an individual wall varies from 60e($7.944\mu m/cm^2$) to 600e($79.44\mu m/cm^2$). In the case of continuum approach, we classify the problems according to the correlation length and steric factor, and considered the four separate cases: 1) zero correlation length and zero steric factor, 2) zero correlation length and non-zero steric factor, 3) non-zero correlation length and zero steric factor, and 4) non-zero correlation and non-zero steric factor. Better understanding of the osmotic pressure of ionic liquids confined inside a nanoslit can be achieved by comparing the results of MD simulation and continuum approach.

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