

Abstract Submitted
for the DFD19 Meeting of
The American Physical Society

Negative Pressure of Ionic Liquids Inside a Nanoslit: Molecular Dynamics Study¹ YU DONG YANG, JUNG MIN OH, IN SEOK KANG, POSTECH — Predicting the force acting on the charged surface is important to prevent deformation or swelling of pores. When the electrostatic interaction between charged pore and its counter-ions is predominant, the internal electrolyte can pull the wall. This means the total pressure becomes negative. Since it becomes complicated to predict with considering the large size and complex shape of ionic liquids, molecular dynamics simulations are conducted to analyze the pressure acting on the nanoslit wall. The pressure change with respect to the slit width under 1 nm scale was analyzed using coarse-grained model, and it is determined by the competition between the contact and electrostatic component of the total pressure. When the slit width is below a double of each ion size, the negative pressure scale is about O (103 atm) and it is 20 to 40 times the bulk osmotic pressure of each ionic liquids. The ion shape or size is related to the magnitude of contact component, but it hardly affects the negative pressure when the electrostatic component is dominant due to the ion re-arrangement in a slit.

¹This work is supported by the National Research Foundation of Korea (No. 2017R1D1A1B05035211) and BK 21 Plus program of Korea.

Yudong Yang
POSTECH

Date submitted: 26 Jul 2019

Electronic form version 1.4