Confinement Effect to Pressure Acting on the Nanoslit Wall: Molecular Dynamics and Continuum Approach

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When an ionic liquid acts as an electrolyte on a porous electrode, it is very important to predict the pressure acting on the pore wall, which is directly related to the stability of the device. When the domain becomes comparable to the ion size, the confinement effect dramatically changes the pressure scale. Here, we computed the pressure acting on the wall varying the nanoslit width using the solvent-free ionic liquid model with the same ion size and symmetric valence, and the results from the MD and continuum model were compared. The confinement effect had a considerable impact on the pressure acting on the wall, which included not only the EDL overlapping but also the discrete effect from the ion layer structure. The latter couldn't be fully interpreted in the continuum model. In the region where co-ion exclusion phenomena dominated, however, both model similarly predict the co-ion exclusion phenomena and negative pressure in a nanoslit. Through the comparison between the MD and continuum model, we found the applicable length scale limits of the continuum model, which has the potential to decrease the calculation cost when designing nanoporous electrode.