Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Dipolar self-consistent field theory for ionic liquids between charged plates: Effects of dielectric contrast between cation and anion under external electrostatic fields[1] ISSEI NAKAMURA, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We develop a new dipolar self-consistent field theory (DSCFT) for both incompressible and compressible ionic liquids under external electrostatic fields. Our theory accounts for the difference between the dipole moments and the molecular volumes of the cation and anion, and the double layer caused by the strong association of the ions with the electrodes. To date, few theoretical studies have considered the dielectric contrast between the cation and anion. Thus, our study focuses on the effect of the dielectric inhomogeneity on the ion distribution and the capacitance. Our theory shows that the capacitance changes with the applied voltage in agreement with experimental observations. Importantly, the dielectric contrast and the difference in molecular volumes between the cation and anion have equal effects on the magnitude of the capacitance. We also consider compressible ionic liquids by developing a hybrid of DSCFT combined with Monte Carlo simulations. We then demonstrate that the hard-core nature of the ions causes oscillations in the density profile and dielectric value near the charged plates. Accordingly, the dielectric constants derived from the classical theories of Onsager and Kirkwood are shown to be gross approximations of the true situation in nanochannels.

[1]National Natural Science Foundation of China (21474112)

Issei Nakamura
Changchun Institute of Applied Chemistry, Chinese Academy of Sciences

Date submitted: 20 Oct 2015 Electronic form version 1.4