Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Explicit water based quasi-continuum approach for electric double layers (EDLs).[1] SIKANDAR Y. MASHAYAK, NARAYANA R. ALURU, Univ of Illinois - Urbana — Electrostatic interactions of interfacial water molecules play a dominant role in determining the distribution of ions in EDLs. Most theories for EDLs are inaccurate because they fail to include molecular effects of water, such as dielectric permittivity variation and ion hydration. On the other hand, a detailed atomic-level study of EDLs using molecular dynamics (MD) simulations can be prohibitively expensive. To address these issues, we propose a multiscale approach to simulate EDLs based on point dipole coarse-grained (CG) water model and an empirical potential-based quasi-continuum theory (EQT), which incorporates the polarization and hydration effects of water explicitly. To reproduce hydration of ions, ion-water CG potentials are developed. We demonstrate EQT for EDL by simulating NaCl aqueous electrolyte confined in slit-like capacitor channels at various ion concentrations and surface charge densities. We show that the ion and water densities from EQT agree well with the reference MD simulations. EQT is not only as accurate as MD but also orders of magnitude faster than MD. Therefore, EQT provides a multiscale framework to accurately model EDLs, which are fundamental to technological applications such as energy storage, water desalination, and biological systems.

[1]This work was supported by AFOSR (Grant No. FA9550- 12-1-0464) and by NSF (Grant Nos. 1264282, 1420882, 1506619, and 1545907). The authors acknowledge the use of the Taub cluster provided by CSE at the University of Illinois.

Sikandar Y. Mashayak
Univ of Illinois - Urbana

Date submitted: 10 Nov 2016 Electronic form version 1.4