Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Continuum-based multiscale approach to predict the structure and theromdynamic properties of confined fluids[1] S.Y. MASHAYAK, N.R. ALURU, Department of Mechanical Science and Engineering, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign — We present a continuum-based theory to predict the structure and thermodynamic properties of fluids confined in multiple length-scales, ranging from few Angstroms to micron length channels. In this work, we introduce a free energy functional for classical DFT (cDFT) based on the empirical potential-based quasi-continuum theory (EQT). EQT is a simple and fast approach to predict the inhomogeneous density and potential profiles of confined fluids, and the results from EQT compare well with MD simulations. Using the density and potential profiles from EQT, we construct a grand potential functional for cDFT. EQT-cDFT based grand potential can be used to predict various thermodynamic properties of confined fluids. Here, we demonstrate applicability of the EQT-cDFT approach by simulating water confined inside slit-like channels of graphene at various thermodynamic states and channel widths. Using EQT-cDFT approach, we calculate the structure and thermodynamic properties of confined water, such as density profiles, adsorption, PMF profiles, surface tension, local pressure profiles, and solvation forces. It is found that the EQT-cDFT results compare well with the reference water MD simulation results.

[1]This research is supported by AFOSR under grant # 11157642 and by NSF under grant # 1264282.

N. R. Aluru
Department of Mechanical Science and Engineering,
Beckman Institute for Advanced Science and Technology,
University of Illinois at Urbana-Champaign

Date submitted: 15 Nov 2013 Electronic form version 1.4