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A multiscale quasi-continuum theory to determine thermodynamic properties of fluid mixtures in nanochannels MOHAMMAD HOSSEIN MOTEVASELIAN, SIKANDAR Y. MASHAYAK , NARAYANA R. ALURU, Univ of Illinois - Urbana — We present an empirical potential-based quasi-continuum theory (EQT) that seamlessly integrates the interatomic potentials into a continuum framework such as the Nernst-Planck equation. EQT is a simple and fast approach, which provides accurate predictions of potential of mean force (PMF) and density distribution of confined fluids at multiple length-scales, ranging from few Angstroms to macro meters. The EQT potentials can be used to construct the excess free energy functional in the classical density functional theory (cDFT). The combination of EQT and cDFT (EQT-cDFT), allows one to predict the thermodynamic properties of confined fluids. Recently, the EQT-cDFT framework was developed for single component LJ fluids confined in slit-like graphene channels [Mashayak, S. Y., M. H. Motevaselian, and N. R. Aluru, Journal of chemical physics 142, 244116 (2015)]. In this work, we extend the framework to confined LJ fluid mixtures and demonstrate it by simulating a mixture of methane and hydrogen molecules inside slit-like graphene channels. We show that the EQT-cDFT predictions for the structure of the confined fluid mixture compare well with the MD simulations. In addition, our results show that graphene nanochannels exhibit a selective adsorption of methane over hydrogen.

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