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Quasi-continuum multiscale theory for confined Lennard-Jones fluid mixture MOHAMMAD H. MOTEVASELIAN, SIKANDAR Y. MASHAYAK, NARAYANA R. ALURU, Univ of Illinois - Urbana — A continuum-based approach is developed to predict the structure of confined multicomponent Lennard-Jones fluids at multiple length-scales, ranging from few angstroms to microns. The continuum approach is based on the empirical potential-based quasi-continuum theory (EQT) that incorporates atomistic detail into a continuum framework such as the Nernst-Planck equation. It can also be used to construct a grand potential functional for classical density functional theories (cDFT). EQT and cDFT combination, provide a simple and fast approach to predict the inhomogeneous density, potential profiles and thermodynamic properties of confined fluids. In this work, we demonstrate EQT-cDFT approach by simulating a mixture of methane and hydrogen inside slit-like channels of graphene. We show that the structure of the confined mixture compares well with MD simulation results.

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