

Abstract Submitted  
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**Multiscale analysis of structure of confined simple fluids** TARUN SANGHI, NARAYANA ALURU, University of Illinois at Urbana-Champaign — We discuss our recently proposed multiscale approach, an empirical potential based quasi-continuum theory (EQT), to predict the equilibrium structure of confined fluids across multiple length scales. In EQT, Nernst-Planck's equation is used to obtain self-consistent concentration and potential profiles of the confined fluid. The robustness, accuracy and computational efficiency of the framework are demonstrated by obtaining concentration and potential profiles of several simple Lennard-Jones type fluids (non-polar, spherical molecules such as Methane, Oxygen, Argon) confined in slit like geometries and comparing the results with molecular dynamics (MD) simulations. The extension of the framework for confined polyatomic fluids (linear rigid chain like molecules such as Ethane and Carbon-dioxide) is also discussed.

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