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Multiscale modeling for confined fluids in open framework materials. JIANZHONG WU, UC Riverside — Open framework materials are a special class of crystalline solids that can be synthesized via modular construction from a wide variety of organic linkers and organometallic or nonmetallic nodes. Whereas enormous developments have been reported in recent years for in silico design of these nanostructure materials with predictable crystallographic topology, accurate prediction of the equilibrium and transport properties of gases and liquids in the micropores of such materials remains a daunting challenge. In this presentation, I will summarize our recent efforts toward developing multiscale procedures that enable customized modeling of confined fluids in open framework materials. Our theoretical development leverages recent advances in applications of quantum and statistical mechanical methods, in particular those based on the density functional theory, to predict the electronic structure, intermolecular interactions, and macroscopic properties of the complex heterogeneous systems.

Jianzhong Wu
UC Riverside

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