148d Bulk and Interfacial Properties of Simple Confined Fluids

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Fluids confined by surrounding walls of any form are defined as confined fluids. Bulk thermodynamic properties and interfacial phenomena of confined fluids in nano and meso scales are important in various industrial processes such as catalysis, chromatography, oil recovery, membrane separation, and lubricant systems. Hence, in recent years confined fluids have been rigorously studied due to their exotic thermodynamic properties and phase behavior as compared to those in bulk fluids. However, little has been done to understand the interfacial phenomena of confined fluids. The effect of wall-fluid interaction is often a difficult target to explore using experimental approaches due to the small dimensions involved. Molecular modeling approach, however, can enhance detailed descriptions at the atomistic level with less hindrance. With this approach, we aim to obtain accurate interfacial properties and understand phase behavior of fluids confined in a form of a slit-pore.

In this study, we investigate interfacial properties and vapor-liquid phase coexistence of square-well and Lennard-Jones fluids in a slit-pore. Molecular dynamics (MD) and grand-canonical transition-matrix Monte Carlo (GC-TMMC) with the aid of histogram reweighting are utilized to obtain properties such as density, pressure, and surface tension. We also examine these properties with respect to width of pore, wall structure, and wall-fluid interaction. The geometry of confinement is simple yet not fully explored with respect to lattice structure of wall and wall-fluid interaction. Therefore, this study will enhance fundamental understanding of confined fluids, enabling the study of realistic systems in the future.