223c Coarse Graining of Molecular Models for Fluids in Porous Materials

Bradd Libby and Peter A. Monson

Coarse-grained lattice models (in which the spacing of lattice sites is the same magnitude as the diameter of the molecules of interest) have been intensively used for decades to study phase transitions in simple fluids and other systems. At length scales comparable to the molecular size, these models impose too much structure on the system and do not adequately sample the range of configurations available to real molecules. On the other hand, off-lattice (or continuum) models require large computational resources when applied to large system sizes. Recently Panagiotopoulos studied models that incorporate intermediate coarse graining and found that, at temperatures near critical, the density of a lattice gas matched the off-lattice equation of state to a small degree of error for ratios of only about 5 or higher [1]. Even results for diameter-to-spacing ratios of 3 are both qualitatively and quantitatively reasonable. In this work, we investigate the usefulness of a lattice model of variable coarse graining for fluids confined in pores. We consider grand canonical Monte Carlo simulation of Lennard-Jones particles confined by walls of slit-like or cylindrical geometry using a sequence of coarse grainings. Our results indicate that the use of intermediate coarse-grained models can be useful for confined fluids also.

[1] A. Z. Panagiotopoulos, J. Chem. Phys., 112, 2000, 7132-7137.