Single Repulsive, Attractive and Amphiphilic Chains in Normal and Associated Supercritical Solvents: Molecular Simulation Study

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Solvent driven changes in chain conformations that occur in normal and associated supercritical solvents have been investigated systematically using simple molecular models. Repulsive and attractive chains are modeled as 10 connected hard-sphere and square-well segments, respectively, and the amphiphilic chain is represented by a diblock chain consisting of five square-well and five hard-sphere segments. The normal solvent is modeled as a square-well fluid and the associated solvent is represented by the extended primitive model of water. Using the configurational-bias Monte Carlo method combined with the parallel tempering technique, we calculate the mean square end-to-end distance and radius of gyration for the single repulsive, attractive and amphiphilic chains over a broad range of densities and temperatures. Subsequently, the coil-to-globule transition temperature at which the chain adopts a quasi-ideal conformation is determined.