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Computational polymer physics: Hard-sphere chain in solvent systems[1] AVINASH GAUTAM, DANIEL GAVAZZI, MARK TAYLOR, Dept. of Physics, Hiram College — In this work we present results for chain conformation in two simple chain-in-solvent systems constructed from hard-sphere monomers of diameter D. The first system consists of a flexible chain of fused hard spheres (i.e., bond length L=D) in a monomeric hard-sphere solvent. The second system consists of a flexible tangent hard-sphere chain (L=D) in a dimeric hard-sphere solvent with L=D. These systems are studied using Monte Carlo simulations which employ both single-site crankshaft and multi-site pivot moves to sample the configuration space of the chain. We report chain structure, in terms of site-site probability functions, as a function of solvent density. In all cases, increasing solvent density leads to an overall compression of the chain. At high solvent density the chain conformation is closely coupled to the local solvent structure and we speculate that incommensurate structures may lead to interesting conformational transitions.

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