

Abstract Submitted
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Local structure in hard-sphere chain-molecule fluids¹ SAMBID WASTI, Dept. of Physics, Hiram College, Hiram OH, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — The conformation of a polymer chain in solvent is coupled to the local structure of the solvent environment. For hard-sphere systems, a monomeric solvent acts to compress a flexible hard-sphere-solute chain and, for a dense system, the local solvent structure is imprinted onto the chain. Here we use Monte Carlo simulation, including bond-rebridging moves, to study the size and conformation of a hard sphere chain in a hard-sphere solvent as a function of both solvent density and solvent diameter. We also study the structure of a hard-sphere-chain solute in a hard-sphere-chain solvent. In the case of a 5-mer chain in 5-mer solvent we show that the effects of solvent can be mapped to a set of two-body solvation potentials. Following our previous work on hard-sphere chains in monomeric solvent [1], we explore the application of these short chain potentials to the study of longer chain-molecule fluids.

[1] M.P. Taylor and S. Ichida, J. Polym. Sci. B: Polym. Phys. 45, 3319 (2007).

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