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Local Structure in Short Chain Molecule Fluids[1] SAMBID WASTI, SUBRAT KHANAL, MARK TAYLOR, Dept. of Physics, Hiram College — The macroscopic properties of materials comprised of polymeric components depend on the underlying local structure or conformation of the constituent polymers. Thus, the viscosity and optical birefringence of a polymeric liquid depend on the degree of entanglement and alignment of the individual polymer chains. Similarly, the functionality of biopolymers is strongly dependent on local chain conformation. Chain conformation itself is determined by both intramolecular interactions and the local solvent environment. Here we use Monte Carlo computer simulation techniques to study local structure in liquids comprised of short flexible chain molecules. We work with a simple pearl-necklace polymer chain model in which the monomers are hard-spheres. We have computed both single chain and chain-chain average structure in pure N-mer liquids with $N \leq 5$ across a range of fluid densities. We have also investigated the conformation of a flexible M-mer chain in a N-mer solvent. Our primary interest in this study has been how solvent architecture (i.e., chain length in this case) affects the conformation of a polymer solute. We are currently developing a solvation potential representation of these molecular solvents which will allow us to map the chain-in-solvent problem to a single chain problem.

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