

Computer Simulation of Self-assembling Material

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The connection between the morphological characterization of single molecule and phase behavior of self-assembled rod-coil triblock copolymer HEMME was studied. Dissipative particle dynamics simulation was carried out to study the mechanism of phase behavior of the solvent-copolymers system. The solvent-induced effect and temperature were found important in the aggregation of block copolymers. The sizes and stabilization energies of mushroom-shaped supramolecular HEMMH clusters were further investigated by molecular modeling method. Clusters of sizes from 16 to 90 molecules were found to be stable. In combination of classical and simple quantum mechanical calculations, the band gaps of HEMME clusters with various sizes were estimated. The band gap was converged at 2.45 eV for cluster contains 90 molecules. Nonlinear optical properties of the material were investigated by the semi-empirical quantum mechanical calculations of molecular dipole moment and hyperpolarizabilities. All simulation results are consistent with experimental observations and give evidence for a general mechanism governing the phase behavior in thin films of modulated phases.