Size Control of Self-Assembled Core-Shell CdSe/ZnS by Dissipative Particle Dynamics

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Size control of quantum-dot has been an important issue due to the sensitive variation of its fluorescent property. The difficulty of the target-size synthesis exists due to the multiplicity of components and becomes more severe when the components make a core-shell form, which also induces interfacial problems. Thus, in this study, the self-assembly of CdSe/ZnS core-shell quantum dot is investigated by dissipative particle dynamics (DPD) method, which has never been tried. We systematically modeled coarse-grained beads representing constituent molecules, which are CdSe, ZnS, trimethylphosphine(TOP), trimethylphosphine oxide(TOPO), water, and hexane, via investigating solubility parameters based on their physical structures. Note that the self-assembly occurs due to phase separations of like and unlike molecules with corresponding affinities. With constant-temperature molecular dynamics simulations, the quantum dots are self-assembled to show different structural tendencies such as columnar, lamellar, and core/shell phases based on compositions of components. We found that the optimal range of the ratios of materials, which decides the size of quantum dots, exists for making the core-shell phase.