Modeling of CdSe/ZnS core/shell Quantum Dot via coarse-graining method

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The synthesis methods of core/shell quantum dot (QD) have been experimentally developed about several decades ago. However, there are still questions on its interfacial behaviors between inorganic shell and ligand shell in atomistic level. Thus, we tackled this problem by the molecular modeling and simulation approach. Especially, a coarse-grained simulation method, which dissipative particle dynamics (DPD), has been chosen for its convenient way of interpreting real chemicals. We computationally mimicked the experimental synthesis process of TOP/TOPO passivated CdSe/ZnS core-shell QD step by step. Coarse-grained beads are modeled with interaction parameters between constituent molecules, which are derived from mixing energy method based on the Flory-Huggins theory. Optimal quantities and ratio of TOP/TOPO on CdSe/ZnS core/shell QD was estimated from various test simulations for colloidal stability of passivated QD under dispersion state in hexane.