Absorption and Binding of Capping Molecules for Highly Luminescent CdSe Nanocrystals - DFT Simulation Studies

Supporting Information

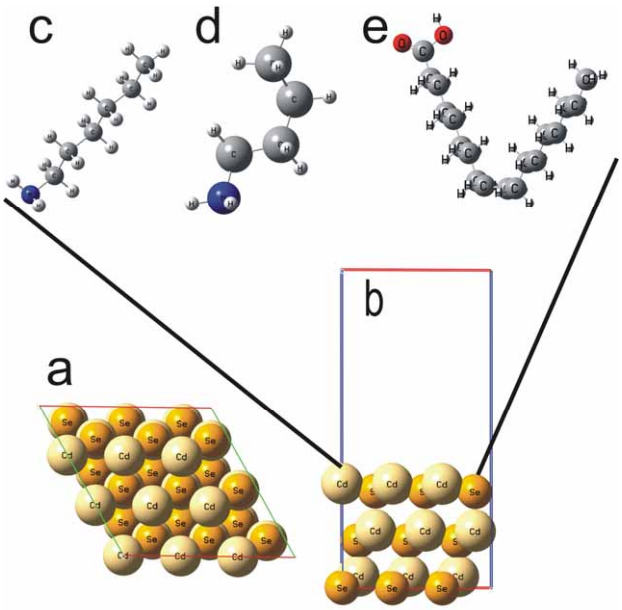

Figure S1. (a) Top view of the CdSe(111) 3 × 3 surface; (b) Side view of the CdSe(111) 3 × 3 slab; DFT optimized geometry of (c) HA; (d) BA; (e) OA molecule.

Density functional theory (DFT) and self-consistent periodic calculations were performed to elucidate the fundamental reasons behind the binding energy and charge analyses of CdSe with *n*-BA, *n*-HA and OA. The periodic slab model comprised a six-layer of CdSe, a 3 × 3 surface supercell with dimensions of 12.940 × 12.940 × 23.924 $Å^3$, separated by a vacuum space of 14 Å. The adsorbed capping molecules in the top CdSe layer were allowed to fluctuate by a given perturbation, while CdSe atoms at the bottom layer remained fixed as the boundary condition. The system would gradually become relaxed to achieve a balanced state with convergent energy, when the forces on the relaxed atoms were less than 0.001 eV/Å.