Structural and electronic properties of bare and capped Cd$_n$Se$_n$/Cd$_n$Te$_n$ nanoparticles ($n = 6, 9$) ALEKSEY KUZNETSOV, Department of Chemistry, Duke University, D. BALAMURUGAN, Department of Chemistry, Indiana University, SPIROS S. SKOURTIS, Department of Physics, University of Cyprus, DAVID N. BERATAN, Department of Chemistry, Biochemistry & Physics, Duke University — Relationships between structures and properties (energy gaps, vertical ionization potentials ($\text{IP}_v$), vertical electron affinities ($\text{EA}_v$), and ligand binding energies) in small capped CdSe/CdTe nanoparticles (NPs) are poorly understood. We have performed the first systematic density functional theory study of the structures and electronic properties of Cd$_n$Se$_n$/Cd$_n$Te$_n$ NPs ($n = 6, 9$), both bare and capped with NH$_3$-, SCH$_3$, and OPH$_3$-ligands. NH$_3$- and OPH$_3$-ligands cause HOMO/LUMO energy destabilization in capped NPs, more pronounced for the LUMOs than for the HOMOs. Orbital destabilization drastically reduces both the $\text{IP}_v$ and $\text{EA}_v$ of the NPs compared with the bare NPs. For SCH$_3$-capped Cd$_6$X$_6$ NPs, formation of expanded structures was found to be preferable to crystal-like structures. SCH$_3$-groups cause destabilization of the HOMOs of the capped NPs and stabilization of their LUMOs, which indicates a reduction of the $\text{IP}_v$ of the capped NPs compared with the bare NPs. For the Cd$_9$X$_9$ NPs, similar trends in stabilization/destabilization of frontier orbitals were observed.

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