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Structural and electronic properties of bare and capped CdnSen/CdnTen 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 (IP_v), vertical electron affinities (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_nSe_n/Cd_nTe_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 IP_v and EA_v of the NPs compared with the bare NPs. For SCH_3-capped Cd_6X_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 IP_v of the capped NPs compared with the bare NPs. For the Cd_9X_9 NPs, similar trends in stabilization/destabilization of frontier orbitals were observed.

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