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Compositional Distribution and Electronic Structure of Ternary Compound Semiconductor Nanocrystals SUMEET PANDEY, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts Amherst, MA 01003 — We present a first-principles-based theoretical study of compositional distribution and the resulting electronic structure of ternary quantum dots (TQDs) of compound semiconductor nanocrystals. The analysis is based on first-principles Density Functional Theory (DFT) calculations of atomic and electronic structure and on Monte Carlo (MC) simulations of compositional distribution according to DFT-parameterized valence force field models. We report results for $ZnSe_{1-x}S_x$ (type-I), $ZnSe_{1-x}Te_x$ (type-II), and $In_xGa_{1-x}As$ (Reverse type-I) TQDs with nm-scale diffusion lengths and large surface-to-volume ratios. The equilibrium compositional distribution is predicted as a function of overall composition (x) and TQD diameter and its impact on the electron density distribution, electronic density of states, and band gap of the TQDs is analyzed. We find that thermodynamically stable atomic distributions allow for optimal band-gap tenability and wave function confinement in TQDs. Our findings explain the possibility for compositional redistribution that may cause, over time, favorable or adverse changes of the TQD electronic properties with far reaching implications for the synthesis and applications of such nanostructures in devices.

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