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Electronic structure and optical spectra of Bulk and Nanocrystalline $CuInS_2$[1] MICHAEL MEHL, ALEXANDER EFROS, Naval Research Laboratory, Washington DC, ANDREW SHABAEV, George Mason University, Fairfax VA — Chalcopyrite $CuInS_2$ is a promising candidate for semiconductor photovoltaic devices. Here we study the behavior of the electronic structure and optical spectra of nanocrystalline $CuInS_2$. We determine the bulk band structure using the HSE06 Hybrid Density Functional as implemented in the Vienna Ab-initio Simulation Package (VASP). We find an equilibrium structure in good agreement with experiment, and a direct band gap of 1.2 eV, as compared to the experimental value of 1.5 eV. The band gap is extremely sensitive to the position of the sulfur atoms, which suggests that it can be controlled in part by the doping of the In site with Ga. $CuInS_2$ is nearly cubic, so we fit the first-principles band structure to a k.p Hamiltonian with invariants consistent with the departure for cubic symmetry. This Hamiltonian is then used to describe the hole spectra in a $CuInS_2$ nanocrystal. We show the symmetry breaking inherent in the chalcopyrite structure can activate the optically passive ground hole state in the nanocrystal, and discuss the resulting optical behavior of the nanocrystal.

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