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Electronic structure of $Cu_{2-x}S$ and related compounds PAVEL LUKASHEV, WALTER R. L. LAMBRECHT, Case Western Reserve Univ., TAKAO KOTANI, MARK VAN SCHILFGAARDE, Arizona State Univ. — Chalcosite Cu_2S and digenite $Cu_{1.8}S$ are possibly interesting semiconductors for photovoltaic applications. Their electronic structure is poorly understood because their crystal structure is complex. If consists of a close-packed lattice of S with mobile Cu occupying various types of interstitial sites with a statistical distribution depending on temperature. As a starting point for understanding these materials, we investigated the simpler antifluorite structure. Both local density approximation (LDA) and self-consistent quasiparticle GW calculations with the full-potential linearized muffin-tin orbital method give a semimetallic band structure with the Fermi level pinned at a degenerate Cu-d band state at Γ. A random distortion of the Cu atoms from the perfect antifluorite positions inside each S cage is found to break the degeneracy of the d state at Γ and thus opens up a small gap of about 0.1 eV in LDA. The experimental evidence for a semiconducting gap of about 1 eV is critically examined. To gain further insight into the Cu d and s-band shifts beyond LDA, we considered other Cu compounds such as Cu_2O and CuBr. We compare their LDA and GW band structures and determined the effective masses and Kohn-Luttinger Hamiltonian parameters for CuBr.

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