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Crystal and Electronic Structure of Copper Sulfides PAVEL LUKASHEV, WALTER R. L. LAMBRECHT, Department of Physics, Case Western Reserve University — Because of the complexity of the crystal structure of $Cu_{2-x}S$, no electronic band structure studies have been performed in the past. These materials have S atoms on a (hcp) or at high-temperature (fcc) close packed lattice but the Cu atoms occupy various low-symmetry Wyckoff sites of which only the statistical distribution is known from X-ray diffraction experiments. Here, we constructed supercell models for the cubic and hexagonal phases with the Cu positions determined by a weighted random number generator. The electronic structure of both these models and the monoclinic structure are studied using the full-potential linearized muffin-tin orbital method in the local density approximation (LDA). Both LDA and GW quasiparticle calculations give a zero band gap for the latter. The supercell models gave small band gaps of order 0.1–0.2 eV. Adding a Cu-s shift as suggested by the antifluorite structure GW calculation and an analysis in terms of atomic orbitals, increases the gap to about 0.5 eV.

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