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Large band gap bowing in CuAgGaS₂ chalcopyrite semiconductors and its effect on optical parameters CHANDRIMA MITRA, Case Western Reserve University, Department of Physics, WALTER LAMBRECHT, Case Western Reserve University, Department of physics — $\text{Cu}_x\text{Ag}_{1-x}\text{GaS}_2$ chalcopyrite semiconductors have been found to exhibit a large band gap bowing. Here we use full-potential linearized muffin-tin orbital calculations in the local density approximation of density functional theory to study the electronic band structure of these materials. The randomness in the alloy is treated by the special quasirandom structures. Some layered ordered compounds are studied as well. We find the band gap to depend strongly on the c/a ratio which varies nonlinearly with concentration, in agreement with experimental data by Matsushita et al. The bowing coefficient is found to be 0.74. We also calculate the indices of refraction and their dependence on concentration. Band gap corrections are adjusted using direct shifts to the conduction bands and adjusted for the end compounds. We find that the nonlinear behaviour of the band gap also leads to a non-linear behaviour of the index of refraction with x .

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