

Abstract Submitted
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Origin of p-type conductivity in wide band gap BaCuQF (Q=S,Se,Te) semiconductors G. SCHNEIDER, A. ZAKUTAYEV, Oregon State University — Bariumcopperchalcogenidefluoride, BaCuQF (Q=S,Se,Te), is a family of p-type wide band gap semiconductors with excellent transparency over the whole visible part of the spectrum. Optical properties can be continuously tuned in thin film solid solutions of BaCuQF. Hole carrier concentration and mobility in BaCuQF decreases from Q = Te→Se→S. Understanding and control of the p-type conductivity in these materials is crucial for potential applications in photovoltaics and transparent electronics. We have investigated the origin of p-type conductivity using ab initio density functional theory in the GGA approximation. The structure and energetics of point defects have been determined using a supercell approach. Cu vacancies are the most likely origin of free hole carriers. Donor like defects such as chalcogen vacancies lead to strong compensation of charge carriers in BaCuSF and BaCuSeF but not BaCuTeF. Hole concentrations obtained from a self-consistent thermodynamic model reproduce the experimental trends. The potential for charge carrier control through intentional doping will be discussed.

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