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First principles study of p-type conductivity in wide band gap Cu_3TaQ_4 (Q=S,Se,Te) semiconductors F.L. BARRAS, A. ZAKUTAYEV, G. SCHNEIDER, Oregon State University — A recent study of Cu_3TaQ_4 (Q=S or Se) has shown that these materials exhibit several favorable optoelectronic properties including large optical band gap, tunable visible photoemission, and p-type conductivity.[1] Cu_3TaQ_4 is unique among wide band gap p-type semiconductors in that it crystallizes in a cubic structure and is expected to show isotropic optical and electronic properties. The origin of p-type conductivity in these materials has been investigated using density functional theory in the GGA approximation. The structure and energetics of point defects have been determined using a supercell approach. We find Cu vacancies to be the most likely origin of free hole carriers. Compensation by donor like defects such as chalcogen vacancies is estimated to be negligible because of high formation enthalpies. Our study suggests that low overall defect concentrations are achievable in Cu_3TaQ_4, raising the potential that these materials could be used for p-type channel transparent transistors.

[1]P.F. Newhouse et al, Thin Solid Films **517**(2009) 2473

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