Abstract Submitted for the MAR07 Meeting of The American Physical Society

Properties of a potential transparent p-type semiconductor $\mathrm{Cu_3TaQ_4}$ (Q = S or Se)¹ PETER HERSH, Department of Chemistry, Oregon State University, PAUL NEWHOUSE, Department of Physics, Oregon State University, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, JANET TATE, Department of Physics, Oregon State University — Physical, optical and electrical properties of powder samples of the $\mathrm{Cu_3TaQ_4}$ (Q = S or Se) series are investigated to determine the potential as a transparent semiconductor. The series crystallizes in a P-43m sulvanite structure. The sulfide has a lattice parameter of a = 5.5036(4) Å and the selenide has a lattice parameter of a = 5.6535(7) Å. The optical band gaps are 2.75eV for $\mathrm{Cu_3TaS_4}$ and 2.36eV for $\mathrm{Cu_3TaSe_4}$. Seebeck coefficients of $+27\mu\mathrm{V/K}$ for $\mathrm{Cu_3TaS_4}$ and $+24\mu\mathrm{V/K}$ for $\mathrm{Cu_3TaSe_4}$ confirm that both materials are p-type. FLAPW band structure calculations indicate that the band gap is indirect.

¹Supported by the National Science Foundation

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Date submitted: 20 Nov 2006 Electronic form version 1.4