Abstract Submitted
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Ab initio search for new p-type transparent conductors among oxide sulfides[1] KANBER LAM, GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, KENNETH POEPPELMEIER, Northwestern University, ALEX ZUNGER, University of Colorado, Boulder — Optimal p-type, i.e., hole-conducting, transparent materials must meet the design metrics of large band gap for transparency, and light hole effective masses and large hole content for good p-type conductivity. The oxide sulfides could potentially satisfy these design metrics better than oxides do, owing to the stronger hybridization between the S p and metal orbitals that can produce a more dispersive valence band maximum (VBM) and lighter hole masses than in oxides. LaOCuS is the prototype p-type transparent conductor (TC) among oxide sulfides. Here, we perform a density functional study of ~ 30 oxide sulfides, based on transition metals and column II and III elements, to identify compounds in this set that meet the design metrics for p-type TCs. We screen these materials using band gaps and hole effective masses. The analysis of the VBM wavefunctions shows that these oxide sulfides can be classified into "band-mixed," with a continuous distribution of the wavefunction on both anions, and "band-segregated," with the VBM mostly originating from one of the anions. The correlation between the type of VBM wavefunction and the O and S arrangement in the material (anion mixed vs. anion segregated) provides a designing criterion for new mixed-anion p-type TCs.

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