

Abstract Submitted  
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**A classification scheme of oxide sulfides to guide the design of new hole-conducting transparent materials**<sup>1</sup> GIANCARLO TRIMARCHI, KANBER LAM, ARTHUR FREEMAN, KENNETH POEPPELMEIER, Northwestern U., Evanston, IL, ALEX ZUNGER, U. of Colorado, Boulder, CO — The addition of S to transition metal oxides has been contemplated as a way to overcome the limitations of pure oxides by producing a hybridized O-S band with lighter hole mass and narrower gap. Here, we show that O-S mixing could lead either to a continuous band broadening and an upward shift of the valence bands (“band amalgamation” scenario) or to the formation of S-localized states deep in the band gap of the host oxide above the O band (“band pinning” scenario). We survey the La-based oxide sulfides by first-principles methods and we observe the following types of VBM wavefunction in relation to the coordination of the O and S atoms: (i) O and S segregate into separate molecular units; the VBM is preferentially localized on the S units (e.g., LaOCuS). (ii) O and S segregate into separate molecular units; the VBM is delocalized on both O and S units (e.g., (LaO)<sub>2</sub>SnS<sub>3</sub>). (iii) O and S are spatially mixed in the lattice; the VBM is preferentially localized on S (e.g., LaGaOS<sub>2</sub>). (iv) O and S are spatially mixed in the lattice; the VBM is delocalized on both S and O (e.g., LaCrOS<sub>2</sub>). Thus, selecting the type of anion coordination is a possible route to tune the hole conductivity in oxide sulfides.

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