Abstract Submitted
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Theory-driven design of hole-conducting transparent oxides[1] G. TRIMARCHI, H. PENG, IM J., A.J. FREEMAN, V. CLOET, A. RAW, K.R. POEPPELMEIER, Northwestern University, Evanston, IL 60208, K. BISWAS, S. LANY, NREL, Golden, CO 80401, A. ZUNGER, University of Colorado, Boulder, CO 80309 — The design of *p*-type transparent conducting oxides (TCOs) aims at *simultaneously* achieving transparency and high hole concentration and hole conductivity in one compound. Such design principles (DPs) define a multi-objective optimization problem that is to be solved by *searching* a large set of compounds for optimum ones. Here, we screen a large set of ternary compounds, including Ag and Cu oxides and chalcogenides, by calculating via first-principles methods the design properties of each compound, in order to search for optimum *p*-type TCOs. We first select Ag_3VO_4 as a case study of the application of *ab-initio* methods to assess a compound as a candidate *p*-type TCO. We predict Ag_3VO_4 (i) to have a hole concentration of $\approx 10^{14}$ cm^{-3} at room temperature, (ii) to be at the verge of transparency, and (iii) to have lower hole effective mass than the prototype *p*-type TCO $CuAlO_2$. We then map the hole effective mass *vs.* the band gap in the selected compounds and determine those that best meet the DPs by having simultaneously minimum effective mass and a band gap large enough for transparency.

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