

Abstract Submitted
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Sulfur-alloyed chromium oxide: A new p-type transparent conducting oxide host¹ SAMIRA DABAGHMANESH, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium, ROLAND SANIZ, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, ERIK NEYTS, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium, BART PARTOENS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — Developing a p-type transparent conducting oxide (TCO) has always been challenging. The main problem of most p-type TCOs is the high effective hole mass, resulting in a low conductivity, brought by a flat valence band. In our work, we introduce sulfur-alloyed Cr_2O_3 as a new TCO host. Using first-principles methods we investigate whether we can increase the valence band dispersion (i.e. reduce the hole mass) by anion alloying with sulfur, while keeping the band gap large enough for optical transparency. We calculate the electronic properties of $\text{Cr}_4\text{S}_x\text{O}_{6-x}$ and consider different alloying concentrations $x=1-5$. We critically examine the accuracy of different density functionals and methods, including PBE, PBE+U, HSE06, as well as perturbative approaches within the GW approximation. Our results demonstrate that $\text{Cr}_4\text{S}_2\text{O}_4$ has an optical band gap of 3.08 eV and an effective hole mass of 1.8 m_e . This suggests $\text{Cr}_4\text{S}_2\text{O}_4$ as a new p-type TCO host candidate.

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