Computational Prediction of an n-type Transparent Conducting Oxide: F-doped Sb_2O_5

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Transparent conducting oxides possess a unique combination of optical transparency and electrical conductivity, making them indispensable in optoelectronic applications. [1] However, the heavy dependence on a small number of established transparent conducting oxides (In_2O_3, SnO_2, ZnO, and Ga_2O_3) places limitations on the number and types of devices they can support. Additionally, the high cost due to the scarcity of rare elements raises concerns about their long-term sustainability and large-scale production. [2] Discovering more wide band gap oxides that can be doped to display metallic-like conductivity is therefore necessary.

In this work, we use the PBE0 hybrid functional to investigate the defect chemistry of the binary Sb(V) system, Sb_2O_5. [3] We observe a large optical band gap over 3.6 eV, enabling transparency. The calculated Sb_2O_5 electronic structure shows a dispersive conduction band minimum, indicating high electron mobility. Although the intrinsic defect study shows that the undoped Sb_2O_5 is insulating, a wide n-type doping window was found to facilitate the introduction of extrinsic dopant, in which a high charge carrier concentration can be obtained. Fluorine was chosen to substitute on the oxygen sites, and the results indicate that the F-doped Sb_2O_5 exhibits degenerate n-type semiconductor behaviour. Our band alignment calculations demonstrate that Sb_2O_5 has a larger electron affinity than the established transparent conductors, which can increase the efficiency of organic solar cell applications. The findings corroborate the potential of Sb(V)-based oxides as alternative earth-abundant n-type TCOs, providing much-needed diversity in the field of transparent conducting materials.

References

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