Extrinsic Doping Mechanism in Sb_2O_5 as a Promising n-type Transparent Conducting Oxide

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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 with low electron effective masses, indicating the potential for high electron mobility. *ShakeNBreak* was used to generate different distortions for finding the groundstate structure, and *Doped* was used to manage all the defect calculations and analysis.[4–6] A rare 4-electron negative-U behaviour was found in the Sb vacancy with an oxygen trimer and split-vacancy configuration formed. Although the intrinsic point defect study shows that Sb_2O_5 does not display metallic-like conductivity, with extrinsic doping of Fluorine (F), Tungsten (W) and Molybdenum (Mo), Sb_2O_5 displays degenerate n-type transparent conducting behaviour. Our band alignment calculations demonstrate that Sb_2O_5 has a larger electron affinity than the established transparent conductors, which can facilitate electron extraction for organic solar cell applications. The findings of this under-explored Sb(V) binary system demonstrate the feasibility and potential for Sb(V)-based materials to be promising transparent conducting oxides.

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