Computational Prediction and Experimental Realisation of New Transparent Conducting Oxides

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Transparent conducting oxides have become ubiquitous in modern optoelectronics. However, the number of oxides that are transparent to visible light and have the metallic-like conductivity necessary for applications is limited to a handful of systems that have been known for the past 40 years. In this work, we use hybrid density functional theory and defect chemistry analysis to demonstrate that tri-rutile zinc antimonate, $ZnSb_2O_6$, is an ideal transparent conducting oxide and to identify gallium as the optimal dopant to yield high conductivity and transparency. To validate our computational predictions, we have synthesized both powder samples and single crystals of Ga-doped $ZnSb_2O_6$ which conclusively show behaviour consistent with a degenerate transparent conducting oxide. This study demonstrates the possibility of a family of Sb(V)-containing oxides for transparent conducting oxide and power electronics applications.