**Computational prediction of Cd2Sb2O7 as a candidate TCO**

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Transparent conducting oxides (TCOs) are central to the field of modern optoelectronics, displaying a unique combination of high electrical conductivity and optical transparency, with applications in touch screens, photovoltaics, LCD and OLED displays, and more. [1] The industry standard for TCOs is Sn-doped In2O3 (ITO), which displays optical transmission greater than 90%, with low resistivity and high carrier mobility. However, indium is expensive and has low earth-abundance. Alternative materials that offer comparable or superior properties using different elements are in high demand. [2,3]

Recently, Sb(V) oxides have emerged as promising candidates. [4,5] Sb(V) possesses the (*n* − 1)*d*10*ns*0 *np*0 electron configuration common to many TCO cations, including In(III) in In2O3, leading to a highly disperse conduction band and a large band gap.[5] The Sb(V) oxides also display three-dimensional connectivity of SbO6 octahedra, creating electron pathways that enable high conductivity. ZnSb2O6 [4] was computationally predicted and experimentally realised as a TCO, and Sb2O5 [5] is predicted to be suitable as well, motivating further exploration of this family of materials.

Cd2Sb2O7 contains Sb(V) and was flagged in a high-throughput study as having a relatively large band gap and low electron effective mass, suggesting possible transparency and conductivity. [6] However, there has been no investigation into the material’s defect chemistry. For these reasons it was decided to investigate Cd2Sb2O7 more thoroughly. The optoelectronic and structural properties of Cd2Sb2O7 were calculated using the hybrid PBE0 functional along with its intrinsic and dopant defect chemistry. Its charge transport was calculated using a combination of ab initio and semi-empirical DFT based methods.

Our results suggest an optical band gap in the transparent range, a high intrinsic electron carrier concentration due to antisite defects, giving high intrinsic mobility and conductivity, and a large doping window, enabling n-type doping to further enhance conductivity. This provides further evidence for the potential of Sb(V) oxides as TCOs.

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