

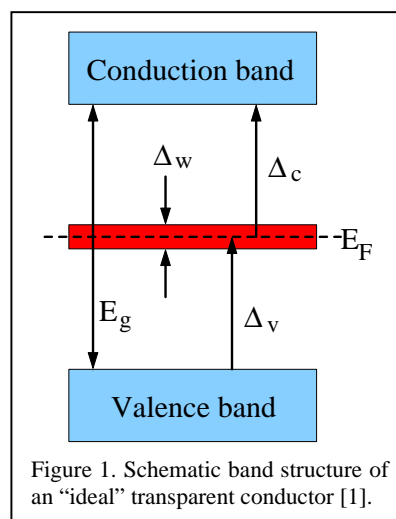
Density Functional Theory: From Conventional to Novel Transparent Conductors

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All well-known and widely used transparent conducting oxides (TCO) – such as In, Sn, Zn, Cd, Ga and Cu oxides and their blends – share similar chemical, structural and electronic properties as well as carrier generation mechanisms. These oxides of post-transition (or transition) metals have a close-packed structure with four or six-fold coordinated metal ions. Upon introduction of native or substitutional dopants, they show high transparency in the visible range and high electrical conductivity. Band structure analysis shows that, common to all known TCO, a highly dispersed band at the bottom of the conduction band is the most important feature of the host electronic band structure. It provides both (i) the high mobility of the carriers due to their small effective masses and (ii) low optical absorption due to a pronounced Burstein-Moss shift which helps to keep the intense interband transitions from the top of the valence band out of the visible range. However, because of the transitions from the partially occupied band at the top of the conduction band, the complete, i.e., 100 % transparency in the visible range can never be achieved in these conventional TCO materials. As a result, complex preparation methods are required to obtain practically useful combination of electrical conductivity and low absorption of visible light since a decrease of the optical absorption comes at a cost of a greatly increased resistance.

Ab-initio methods based on density-functional theory help not only to understand the complex phenomenon but also to predict ways to designing novel materials with desired characteristics. Thorough band structure analysis of the conventional TCO materials suggests an approach to combine 100% optical transparency with high electrical conductivity [1]. The schematic band structure of such an “ideal” TCO is shown in Fig. 1. The introduction of a *deep* impurity band in the band gap of an insulating material would help to keep intense interband transitions (from the



valence band to the impurity band, Δ_v , and from the impurity band to the conduction band, Δ_c) above the visible range, i.e., Δ_v and $\Delta_c > 3.1$ eV. This requires the band gap of a host material to be more than 6.2 eV. Furthermore, the impurity band should be narrow enough ($\Delta_w < 1.8$ eV) to keep intraband transitions (as well as the plasma frequency) below the visible range.

In search for the “ideal” TCO, we studied several materials which satisfy the above set of requirements. In sharp contrast to the conventional TCO with close-packed structure, nanoporous materials, e.g., zeolites, offer a way to incorporate a large concentration of impurities (that ensures good electrical conductivity) without any significant changes in the band structure of the host material, i.e., without compromising the optical transparency.

[1] J.E. Medvedeva, and A.J. Freeman, *Europhys. Lett.* **69**, 583 (2005).