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Transparent Conductors: Understanding and Optimization¹

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The unique combination of two mutually exclusive properties – optical transparency and electrical conductivity – is known to be a prerogative of only a few oxides of post-transition metals, namely, In_2O_3 , ZnO , CdO and SnO_2 . Advances in theoretical understanding of the underlying physical phenomena in conventional transparent conducting oxides (TCOs) and rapid development of the technologies for which TCO is a vital component, stimulate further research aimed at (i) broadening the range of the electronic and optical properties of application-specific transparent conductive materials in a controllable way; (ii) improving the functional capabilities and efficiency of TCOs in a device; and (iii) designing novel materials as a viable, inexpensive alternative to conventional TCOs. Here, we employ first-principles density-functional approach to investigate the structural, electronic and optical properties of several classes of transparent conductors including conventional single-cation main-group oxides, multi-component binary and ternary oxides, as well as several non-oxide materials. Systematic comparative investigations allow us to determine the role of the crystal structure, chemical composition and carrier generation mechanisms on the resulting optical and electronic properties and predict ways to optimize the properties.

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