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Fundamental limits on transparency: first-principles calculations of absorption[1]

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Transparent conducting oxides (TCOs) are a technologically important class of materials with applications ranging from solar cells, displays, smart windows, and touch screens to light-emitting diodes. TCOs combine high conductivity, provided by a high concentration of electrons in the conduction band, with transparency in the visible region of the spectrum. The requirement of transparency is usually tied to the band gap being sufficiently large to prevent absorption of visible photons. This is a necessary but not sufficient condition: indeed, the high concentration of free carriers can also lead to optical absorption by excitation of electrons to higher conduction-band states. A fundamental understanding of the factors that limit transparency in TCOs is essential for further progress in materials and applications. The Drude theory is widely used, but it is phenomenological in nature and tends to work poorly at shorter wavelengths, where band-structure effects are important. First-principles calculations have been performed, but were limited to direct transitions; as we show in the present work, indirect transitions assisted by phonons or defects actually dominate. Our calculations are the first to address indirect free-carrier absorption in a TCO completely from first principles. We present results for SnO_2 [1], but the methodology is general and is also being applied to ZnO and In_2O_3. The calculations provide not just quantitative results but also deeper insights in the mechanisms that govern absorption processes in different wavelength regimes, which is essential for engineering improved materials to be used in more efficient devices. For SnO_2, we find that absorption is modest in the visible, and much stronger in the ultraviolet and infrared.

[1] H. Peelaers, E. Kioupakis, and C.G. Van de Walle, Appl. Phys. Lett. **100**, 011914 (2012).

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