MAR16-2015-002287

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Limits of transparency of transparent conducting oxides[1]

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A fundamental understanding of the factors that limit transparency in transparent conducting oxides (TCOs) is essential for further progress in materials and applications. These materials have a sufficiently large band gap, so that direct optical transitions do not lead to absorption of light within the visible spectrum. Since the presence of free carriers is essential for conductivity and thus for device applications, this introduces the possibility of additional absorption processes. In particular, indirect processes are possible, and these will constitute a fundamental limit of the material. The Drude theory is widely used to describe free-carrier absorption, but it is phenomenological in nature and tends to work poorly at shorter wavelengths, where band-structure effects are important.

We will present calculations of phonon- and defect-assisted free-carrier absorption in a TCO completely from first principles [1]. We will focus in detail on SnO_2, but the methodology is general and we will also compare the results obtained for other TCO materials such as In_2O_3. These calculations provide not just quantitative results but also deeper insights in the mechanisms that govern absorption processes, which is essential for engineering improved materials to be used in more efficient devices.

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

[1]This work was performed in collaboration with E. Kioupakis and C.G. Van de Walle and was supported by ARO and NSF.