Abstract Submitted
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First-principles calculation of indirect absorption in transparent conducting oxides[1] HARTWIN PEELAERS, University of California - Santa Barbara , EMMANOUIL KIOUPAKIS, University of Michigan, CHRIS G. VAN DE WALLE, University of California - Santa Barbara — Transparent conducting oxides (TCOs) are a technological important class of materials that combine high electrical conductivity with transparency in the visible light spectrum. The most frequently used material is Sn-doped In_2O_3, also called ITO. The Sn doping provides the free carriers required for the conductivity. The transparency of the material can be attributed to the fact that direct absorption processes, either across-the-gap or by direct free-carrier absorption, require energies larger than that of visible light photons. But light absorption can still occur due to indirect free-carrier absorption, which is usually described by a phenomenological Drude model. To improve the fundamental understanding of the processes limiting the transparency in these materials, we use a fully first-principles methodology based on density functional theory [1]. We will discuss the importance of phonon- and defect-assisted absorption and compare the results for ITO with our earlier results for SnO_2 [1].

[1] H. Peelaers, E. Kioupakis, and C.G. Van de Walle, Phys. Rev. B 92, 235201 (2015).

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