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Fundamental limits on optical transparency of transparent conducting oxides: free-carrier absorption in \mathbf{SnO}_2^1 HARTWIN PEELAERS, Materials Department, University of California, Santa Barbara, California, EM-MANOUIL KIOUPAKIS, Materials Department, UC Santa Barbara, California; Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California — Transparent conducting oxides (TCOs) are a technologically important class of materials used as transparent contacts in optoelectronic devices, such as flat-panel displays, touch screens, solar cells, and light-emitting diodes. These applications are possible because the TCOs combine high electrical conductivity with transparency to visible light. However, the large concentration of free electrons introduces a source of absorption that forms a fundamental limit to the transparency. We evaluated the importance of phonon-assisted free-carrier absorption in SnO_2 completely from first principles. We also provide insight into the mechanisms that govern absorption in different wavelength regimes. Our results show that the absorption is weak in the visible, but it increases by as much as a factor of 5 in the UV. For the infrared region, we show that the absorption increases with the wavelength, and that this increase is proportional to the third power of the wavelength. We also explain this third power dependency.

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