

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Ab initio calculation of indirect light absorption by free carriers in transparent conducting oxides¹ HARTWIN PEELAERS, EMMANOUIL KIOUPAKIS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Phonon-assisted absorption of light by free carriers is an important optical process in many materials and a challenging problem for computational condensed-matter physics. As transparent conducting oxides play an important role as contacts to light emitters and photovoltaic devices, it is important to consider not only the optical absorption across the band gap, but also the absorption by free carriers due to indirect processes mediated by phonons and defects. Here we calculate these losses using a full ab initio methodology as opposed to a phenomenological Drude model containing empirical parameters. These calculations involve the electron-phonon coupling matrix elements, which are dominated by the longitudinal optical phonon modes. We also compare with the Fröhlich model, which describes the electron-phonon matrix elements in the long-wavelength limit.

¹This work was supported by DOE, the UCSB SSLEC, and the BAEF.

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Date submitted: 26 Nov 2010

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