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Interband and polaronic excitations in YTiO3 from first principles[1] BURAK HIMMETOGLU, ANDERSON JANOTTI, LARS BJAALIE, CHRIS G. VAN DE WALLE, University of California Santa Barbara — $YTiO_3$, as a prototypical Mott insulator, has been the subject of numerous experimental investigations of its electronic structure. The onset of absorption in optical conductivity measurements has generally been interpreted as due to interband transitions at the fundamental gap. Here we re-examine the electronic structure of $YTiO_3$ using density functional theory with either a Hubbard correction (DFT+U) or a hybrid functional. Interband transitions are found to be much higher in energy than the observed onset of optical absorption. However, we show that the holes in the lower Hubbard band tend to become self-trapped in the form of small polarons, localized on individual Ti sites. Exciting electrons from the occupied lower Hubbard band to the small-polaron state then leads to broad infrared absorption, consistent with the onset in the experimental optical conductivity spectra.

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