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**The impact of small polarons on the properties of rare-earth titanates**[1] CHRIS VAN DE WALLE, LARS BJAALIE, BURAK HIMMETOGLU, ANDERSON JANOTTI, Materials Department, Univ. of California - Santa Barbara — Optical conductivity measurements are frequently applied to determine the band gaps of complex oxides, such as the rare-earth titanate ($RTiO_3$) Mott insulators. The onset of the measured spectra, in the range of 0.2-0.7 eV, is commonly interpreted as the Mott-Hubbard gap. However, first-principles calculations that take strong electron-electron interactions into account [using either density functional theory (DFT) with a hybrid functional or DFT+U] produce band gaps close to 2 eV for $GdTiO_3$ and $YTiO_3$ [Himmetoglu et al., Phys. Rev. B 90, 161102 (2014)]. This raises the question of the origin of the absorption below 2 eV observed in optical experiments. We attribute this signal to excitation of small hole polarons. The rare-earth titanates commonly exhibit unintentional p-type conductivity, and we show that hole localization in the form of small polarons is energetically favorable. Configuration-coordinate diagrams enable us not only to assess the peak in optical absorption, but also to model the lineshape. Good agreement with experiment indicates that the infrared absorption is indeed likely to be polaron-related in $GdTiO_3$. The results probably apply to other rare-earth titanates as well.

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