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Point defects, impurities, and small hole polarons in $GdTiO_3$ LARS BJAALIE, University of California, Santa Barbara, ANDERSON JANOTTI, University of Delaware, KARTHIK KRISHNASWAMY, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — $GdTiO_3$(GTO) has become the focus of great interest because of its use in complex-oxide heterostructures that display two-dimensional electron gases with unprecedented high densities. GTO is a Mott insulator, with a band gap arising within the partially filled Ti $3d$ band due to strong electron-electron interactions. GTO often displays hole conductivity, likely attributed to defects or impurities, yet the cause of this unintentional conductivity has not yet been explored. We therefore used density functional theory with a hybrid functional to study their electronic structure. Among native defects, the cation vacancies have the lowest formation energies in oxygen-rich conditions, and oxygen vacancies have the lowest formation energy in oxygen-poor conditions. Among the impurities, r_{Gd}, H_i and C_O have the lowest formation energies. The defects and impurities are intrinsically stable only in a single "natural" charge state, to which various numbers of hole polarons can be bound, which explains the frequent observation of p-type hopping conductivity in the rare-earth titanates. These small hole polarons also lead to optical absorption and act as electron traps in devices.

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