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Small polaron characteristics of the OH center in TiO_2[1]

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Most insulating crystals have nearly-free-electron conduction bands and corresponding conduction properties, with the effective mass increased slightly by large-polaron effects. In TiO_2, the lowest conduction bands contain considerable admixture of Ti 3d states. In this case the conduction electrons become localized, or self-trapped, into small-polaron states [1], and their conduction properties differ considerably from the usual case. EPR experiments by Halliburton *et al.* [2] have shown that this self-trapping is also present in association with point defects, namely substitutional F and interstitial H (which forms a bond with a lattice O). In each case the spin of the unpaired electron is localized on a nearest neighbor Ti. Infrared absorption experiments as a function of temperature on the OH center by Bekisli *et al.* [3] have resolved apparent inconsistencies in the model used to fit earlier IR data. Through detailed analysis they have interpreted their results in terms of a small polaron model which involves several configurations corresponding to the localization of the OH electron on different Ti sites, each of which yields an IR line of slightly different frequency. These conclusions are supported by theoretical results in the literature and by our calculations using the CRYSTAL06 code [4] with a hybridized DFT Hamiltonian.

[1] A. Yidiz *et al.*, J. Appl. Phys. **108**, 083701 (2010).
[2] S. Yang and L. E. Halliburton, Phys. Rev. B **81**, 035204 (2010); A. T. Brant *et al.*, J. Appl. Phys. **110**, 053714 (2011).
[3] F. Bekisli *et al.*, Phys. Rev. B **86**, 155208 (2012).
[4] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

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