Abstract Submitted
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Hybrid functional calculations for defects in TiO_2[1] CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, JOEL VARLEY, Department of Physics, University of California, Santa Barbara, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara — Density functional theory (DFT) has proven its value as an immensely powerful tool for assessing structural properties of defects in semiconductors or insulators. Frequently, however, information about electronic structure is required, i.e., the position of defect levels in the band gap. Since DFT in the LDA or GGA severely underestimates the band gap, the position of defect levels is subject to large error bars. Here we show that the use of hybrid functionals allows us to overcome this problem. We illustrate the power of the approach with the example of point defects in TiO_2, a material of high interest for electronics, optoelectronics, and photocatalysis. Unintentional n-type conductivity in TiO_2 has often been attributed to oxygen vacancies (V_O). We find that V_O is indeed a shallow donor [1]. Our calculated formation energies allow us to assess whether vacancy concentrations are consistent with experimental observations of unintentional conductivity.

[1] A. Janotti, J. B. Varley, P. Rinke, N. Umezawa, G. Kresse, and C. G. Van de Walle, Phys. Rev. B 81, 085212 (2010).

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