Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Small polarons and their interaction with donor centers in Titania[1] ANDERSON JANOTTI, Materials Department, University of California Santa Barbara, CESARE FRANCHINI, University of Vienna and Center for Computational Materials Science, JOEL VARLEY, Materials Department, University of California Santa Barbara, GEORG KRESSE, University of Vienna and Center for Computational Materials Science, CHRIS VAN DE WALLE, Materials Department, University of California Santa Barbara — The use of TiO_2 in photocatalysis, photosensitized solar cells, and memristors strongly depends on the behavior of conduction-band electrons, prompting a more profound understanding of conduction mechanisms. The reported results for the behavior of excess electrons in TiO_2 are contradictory. High carrier mobilities, characteristic of delocalized electrons, have been observed in Hall measurements, whereas optical spectra indicate the presence of localized, small polarons. Using first-principles calculations based on a hybrid functional we study the formation of small polarons, comparing it to delocalized electrons in the conduction band of TiO_2. From the calculated configuration coordinate diagram and migration energy barriers, we discuss the coexistence of small polarons with delocalized electrons, and address how the observed behavior depends on the type of experiment being conducted. The interaction of small polarons with intrinsic defects such as the oxygen vacancy and donor impurities will also be discussed.

[1]This work was supported by NSF, ARO, and by the Austrian FWF.

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Date submitted: 17 Nov 2012 Electronic form version 1.4