

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

Sorting Category: 02.8.1 (C)

**Oxygen vacancies and titanium interstitials in rutile and anatase**<sup>1</sup> JOHN JAFFE, MICHAEL HENDERSON, Pacific Northwest National Laboratory — Native point defects in reduced TiO<sub>2</sub>, namely the oxygen vacancy and Ti interstitial, were investigated computationally for both the rutile and anatase structures. The generalized gradient approximation to density functional theory was used along with a plane-wave expansion and ultrasoft pseudopotentials. Defect formation energies were calculated after geometry relaxation from O vacancies created in the bulk rutile and anatase lattices, from the experimental Ti interstitial position in rutile, and from several trial initial geometries for the Ti interstitial in anatase. Contrary to traditional assumptions but consistent with much recent evidence, the Ti interstitial was found to be predominant over the O vacancy in rutile under most conditions. Donor ionization energies in rutile were consistent with experiment. Surprisingly, the calculations also indicate a dominant role for the Ti interstitial in anatase (lower formation energy than the O vacancy, though not by as much as in rutile, and much shallower ionization levels.) We evaluate these findings against experimental data on pure n-type TiO<sub>2</sub>, and discuss possible implications for transition metal cation doping as well as anion doping of TiO<sub>2</sub>.

<sup>1</sup>Supported by US Department of Energy, Basic Energy Sciences

Prefer Oral Session  
 Prefer Poster Session

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Date submitted: 02 Dec 2005

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