Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Nitrogen-doped TiO_2 for visible light photocatalysis JOEL VARLEY, Department of Physics, University of California Santa Barbara, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California Santa Barbara — Using first-principles calculations we investigate the effects of nitrogen doping on the photocatalytic properties of rutile TiO_2. We find that N can be incorporated into the bulk with appreciable solubility in the form of a substitutional or N_2 split-interstitial defect. Substitutional N gives rise to a deep-acceptor state, while the split-interstitial behaves as a donor. We confirm that substitutional N on the O site is found to effectively lower the absorption of light to the visible-range by approximately 0.6 eV with respect to the bandgap of 3.1 eV, in good agreement with recent experiments. Our results indicate that the N_2 split-interstitial defects do not to contribute to the observed onset of visible-light absorption yet can potentially play a role in the pinning of the Fermi Level. We conclude that N is a good dopant choice for TiO_2, increasing the versatility of TiO_2 for use as a photocatalyst for sub-UV illumination. This work was supported by the NSF MRSEC Program under Grant No. DMR05-20415.

Joel Varley
University of California Santa Barbara

Date submitted: 18 Nov 2009 Electronic form version 1.4