

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Bandgap engineering of rutile with substitutional nitrogen JOHN JAFFE, MICHAEL HENDERSON, Pacific Northwest National Laboratory — TiO_2 in both the rutile and anatase structures has been proposed as an absorber of sunlight for photocatalytic processes, including water splitting to produce hydrogen from solar energy. However, the large band gap of TiO_2 , about 3.0 eV, permits the use of only a small part of the solar spectrum. Alloying with other elements, and especially anion doping with nitrogen, sulfur or other anions in place of oxygen, has shown promise for reducing the band gap of the material, permitting more of the solar spectrum to be used so that photocatalysis with TiO_2 can be made more efficient. However, little is known about the concentration dependence of the bandgap reduction, or about autocompensation of nonisovalent dopants by native defects such as the oxygen vacancy. We have calculated defect formation energies and changes in the DFT bandgap for rutile $\text{TiN}_x\text{O}_{2-x}$ for $x = 0.042, 0.083, 0.167$ and 0.25 . The band gap initially decreases with increasing x , but the reduction largely saturates at about 0.3 eV for $x \geq 0.083$. We also report preliminary results on the formation energy and electronic structure of O vacancies in $\text{TiN}_x\text{O}_{2-x-\delta}$, and on interactions and complexes of these defects.

John Jaffe
Pacific Northwest National Laboratory

Date submitted: 23 Nov 2004

Electronic form version 1.4