

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Fe doping and anion defects in bismuth pyrochlore photocatalysts¹ CEDRIC MAYFIELD, DAVID BARKER, Physics Department, University of Texas Arlington, VAIDYANANTHAN SUBRAMANIAN, Chemistry and Engineering Department, University of Nevada, MUHAMMAD HUDA, Physics Department, University of Texas Arlington — To understand the change in photocatalytic properties of $\text{Bi}_2\text{Ti}_2\text{O}_7$ after incorporating localized Fe 3d electrons, the electronic properties and formation energies of anion defects and cation substitutions have been systematically studied by first principles density functional theory. We have found for each type of doping, intrinsic or extrinsic, structural distortions are localized to the defect site. For the intrinsic defects, O vacancies (O_{vac}) are relatively shallow donors compared to O interstitials (O_{int}). For the extrinsic defects, Fe substitutions at the Bi sites (Fe_{Bi}) are more stable than Fe substitutions at the Ti sites (Fe_{Ti}), however they both promote the acceptor defect levels which are critical for band gap engineering. Complex doping (combined intrinsic and extrinsic doping) was also considered to examine the defect correlations at first nearest neighbor to third nearest neighbor distances. A detailed electronic structure analysis will be presented for both pristine and doped $\text{Bi}_2\text{Ti}_2\text{O}_7$.

¹National Science Foundation

Cedric Mayfield
Physics Department, University of Texas Arlington

Date submitted: 15 Nov 2013

Electronic form version 1.4