Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Red Shifted Absorbance of A-site Substituted Bismuth Titanate Pyrochlore: Characterization and Stability Analysis from First Principles[1] CEDRIC MAYFIELD, MUHAMMAD HUDA, Department of Physics, University of Texas at Arlington — Transition metal inclusion has enhanced photocatalytic activity of bismuth titanate (Bi2Ti2O7) up to an impurity threshold concentration. Beyond the threshold, spectral absorbance is continually red shifted but increased photocurrent is not reciprocated. We investigated, from first principles, the origin of decreased photocurrent in modified Bi2Ti2O7 (BTO) by calculating the electronic structures of a representative set of doping configurations and by performing a phase stability analysis of the doping. We report our theoretical/computational strategy of analyzing free energy space and show an explicit dependence of pure phase synthesis on changes in free energy. Also, we present a probability distribution of the doping configurations based on formation enthalpy to better understand the nature of doping in BTO. We found that transition metal substitutions are favorable at the A-sites due to unchanging coordination with O ions.

[1]This work is supported by National Science Foundation, award no. 1133672.

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Date submitted: 12 Nov 2014 Electronic form version 1.4