Abstract Submitted
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Density functional theory (DFT) study of the electronic structure of $Bi_2O'Ti_2O_6$ for hydrogen production by water splitting[1] DAVID BARKER, CEDRIC MAYFIELD, Physics Department University of Texas at Arlington, VAIDYANATHAN SUBRAMANIAN, Chemical and Materials Engineering, University of Nevada, Reno, MUHAMMAD HUDA, Physics Department University of Texas at Arlington — BTO pyrochlore ($Bi_2O'Ti_2O_6$) is a promising photocatalyst material for hydrogen production by water-splitting. Study of such materials is crucial for the understanding of energy conservation, and to better understand the optical and electronic properties of pyrochloric materials. However, BTO's electrical and optical properties have not yet been studied in greater detail. In this study, density functional theory (DFT) was used to calculate the volume of the cell as well as the energy, and as a result of this calculation the most stable crystal structure was determined. In addition, previous studies have indicated that Fe doped BTO has preferable electronic structure as a photocatalyst. Here, this is studied in depth by placing Fe at different sites in BTO and observing how electronic properties are affected. For example, through the study of the band structure for both BTO and Fe doped BTO; band gaps and the nature of the gaps will be presented, as well as the optical properties of both systems. Examination of the solubility of Fe in different sites of BTO, the most stable structure for Fe doped BTO, the formation energy and the contributions of the different atoms orbitals on the total band structure will be presented as well.

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