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Determining the Stability Zone for Single Phase Synthesis of Fe doped Bismuth Titanate Water-Splitting Photocatalysts[1] CEDRIC MAYFIELD, MUHAMMAD HUDA, Department of Physics, University of Texas at Arlington — Due to their ferroelectricity, high dielectric constant and excellent photocatalyitic properties bismuth titanate (BTO) polymorphs comprise an assortment of phenomenological wide band gap semiconductors that are used in everything from device applications to discoloration of organic pollutants. Recently, the potential for BTO as a high performance water-splitter has gathered serious attention. Without modification BTO already reduces water molecules upon UV irradiation. The band alignment is such that merely increasing the density of states will not only raise the Fermi level closer to the oxidation potential of water, but also reduce the band gap so that its photocatalytic property can be activated by visible light. Unfortunately, engineering the bands of BTO by inclusion of dopants is stifled by a phase transition-prone chemical potential landscape. We have performed a DFT study pertaining to substitutional Fe doping of the cubic pyrochlore phase (Bi2Ti2O7). We aimed to understand the correlation effects that lead to an experimentally observed Fe doping threshold concentration. We found that different precursor materials had significant effects on single phase synthesis of BTO. We present the formation energy analysis of Fe doping configurations that aided in identification of the configurations associated with formation of secondary phases. We conclude that maintaining our proposed conditions for single phase synthesis will increase the Fe doping threshold and simplify the design of an enhanced BTO alloy.

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