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Bandgap properties of amorphous TiO2 (aTiO2) M. KYLEE UNDERWOOD, West Virginia University, BINAY PRASAI, BIN CAI, DAVID A. DRABOLD, Ohio University, JAMES P. LEWIS, West Virginia University — In photocatalytic and photovoltaic applications, TiO_2 is a convenient material due to its stability, abundance, and functionality. The natural bandgap of TiO_2 is very wide thus limits its usability to the UV region of the solar spectrum. Previous research has indicated that these limitations may be overcome by doping with anionic nonmetal elements such as carbon or nitrogen. However, both experimental and theoretical research suggests that these dopants tend to act more as recombination centers rather than truly enhance the functionality of TiO_2. Although naturally occurring in crystalline form, the initial processing of TiO_2 for the production of thin films and powders results in mostly amorphous materials and further processing locks the material into a particular crystalline or poly-crystalline form. The properties of anatase and rutile crystalline structures of bulk and nanophase TiO_2 have been studied in detail; however, amorphous TiO_2 ($aTiO_2$) lacks a similar depth of study. We show, through ab initio density functional theory calculations, that $aTiO_2$ exhibits a bandgap almost identical to crystalline TiO_2. We will further discuss our results for anionic nonmetal dopants in $aTiO_2$.

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