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Analysis of Quasiparticle Energy Band Shifts Resulting from Introduction of Nitrogen into Titanates WEI KANG, Center for Funtional Nanomaterials, Brookhaven National Laboratory, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Laboratory — Titanium oxides and many titanates, such as rutile (TiO_2) and $SrTiO_3$, are promising in photo-catalysis for water splitting and photo-degradation of hazardous materials in the environment, although their large band gaps limit utilization of the solar spectrum to the UV region. Experiments show that introduction of nitrogen by various means can significantly affect the band gap. However, catalytic action also depends on individual conduction and valence band alignments. We address these issues by performing theoretical calculations of the energy spectrum for titanium oxides, titanates and various structures introducing nitrogen into the crystals using the GW method. In contrast to density functional theory approaches, the GW method generally leads to energy levels and band gaps that agree well with experiments. We here use this approach to illustrate the mechanism of band shifting in titanates due to the introduction of nitrogen, in particular the differences in correlation effects for nitrogen related energy bands in these materials. This work is supported by the DOE.

Wei Kang
Center for Funtional Nanomaterials, Brookhaven National Laboratory

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