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Second generation photocatalytic materials - anion doped TiO_2
JAMES LEWIS, HAO WANG, Brigham Young University — TiO_2 is a wide-band gap semiconductor with band gap of 3.0 eV. Recently an effective photoresponse in the visible-light region has been observed in anion doped TiO_2, which is a promising second generation photocatalyst. We contribute a theoretical understanding of this phenomenon. Our ab initio density functional theory investigations show that substitutional anion dopants incorporated into TiO_2 drastically affect the electronic structure of the material thus improving its photoactivity. The resulting smaller bandgaps (in the visible) predicted in this work agrees with the available experimental observations for larger anion concentrations around 5%. We also address the effects of doping concentration on the photoresponse of this material.

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