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Effects of dopant states on the electronic structures in tungsten doped TiO_2 HAO WANG, JAMES LEWIS, Brigham Young University — Despite the broad range of applicabilities for TiO_2 as a photocatalytic material, only about 3% of the solar spectrum (ultraviolet) can be utilized due to its wide intrinsic band gap. Therefore, considerable efforts have been made to extend the photoresponse of TiO_2-based systems further into the visible-light region using dopants. In this work, we explore the electronic structures of tungsten doped TiO_2 using an *ab-initio* tight-binding method, called FIREBALL, which is based on density functional theory (DFT) with nonlocal pseudopotentials within the local density approximation (LDA). Our calculations provide an initial glance into electronic properties required for acceptable photocatalysis.

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