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Atomic structure, electronic properties, and band offsets of $SrRuO_3/TiO_2$ heterojunctions NAHEED FERDOUS, ELIF ERTEKIN, Univ of Illinois - Urbana — Photocatalytic water splitting by sunlight can in principle be an environmentally green approach to hydrogen fuel production, but at present photocatalytic conversion efficiencies remain too small. In titanium dioxide (TiO_2), the most commonly used photocatalyst, the biggest limitation arises from poor absorption of visible light. One way to increase the visible light absorption is to create a composite heterojunction by integrating TiO_2 with a strongly light absorbing material. Inspired by experimental results demonstrating good light absorption in the correlated metal oxide Strontium Ruthenate ($SrRuO_3$), as well as enhanced photocatalytic activity of $SrRuO_3/TiO_2$ heterojunctions [1], we have carried out electronic structure calculations based on density functional theory to explain and improve on the observed properties of such heterojunctions. Our calculations present that this heterojunction exhibits type-II band alignment which is necessary to transport optically excited electrons from the $SrRuO_3$ to the TiO_2, with calculated work functions in good agreement with experimental measurements. Also, DFT calculations help to explain the origin of large light absorption in the correlated metal oxide, which arises from electronic excitations from O 2p levels into the Ru d-orbital quasiparticle states in the material. The use of correlated metal oxide/ TiO_2 heterojunctions is a potentially interesting approach to improved photocatalytic activity. [1] Lee, S, Apgar, B A, & Martin, L W. (2013). Strong visible-light absorption and hot-carrier injection in tio2/srruo3heterostructures. Advanced energy materials, 3(8), 1084-1090.

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