

## Effect of polaronic charge transfer on band alignment at the Cu/TiO<sub>2</sub> interface

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We present a first principles investigation into the electronic properties of an extended interface between rutile TiO<sub>2</sub> and Cu. We show that owing to the highly polarizable nature of TiO<sub>2</sub>, the interface is unstable to the spontaneous formation of small electron polarons at the interface. The resulting dipole leads to an increase in the conduction band offset by 0.4 eV and the presence of a band of occupied states related to Ti d states 1.4 eV below the Fermi energy. This effect should be expected more generally at interfaces between highly polarizable oxides and metals but is missed by standard first principles approaches. Given the ubiquitous nature of such interfaces, this previously overlooked effect may have important implications for diverse applications across science and technology.

[1] K P. McKenna, *Phys. Rev. B* **in press**, - (2016).