

Supplementary Information

Schottky barrier and band edges engineering via interfacial structure and strain for Pt/TiO₂ heterostructure

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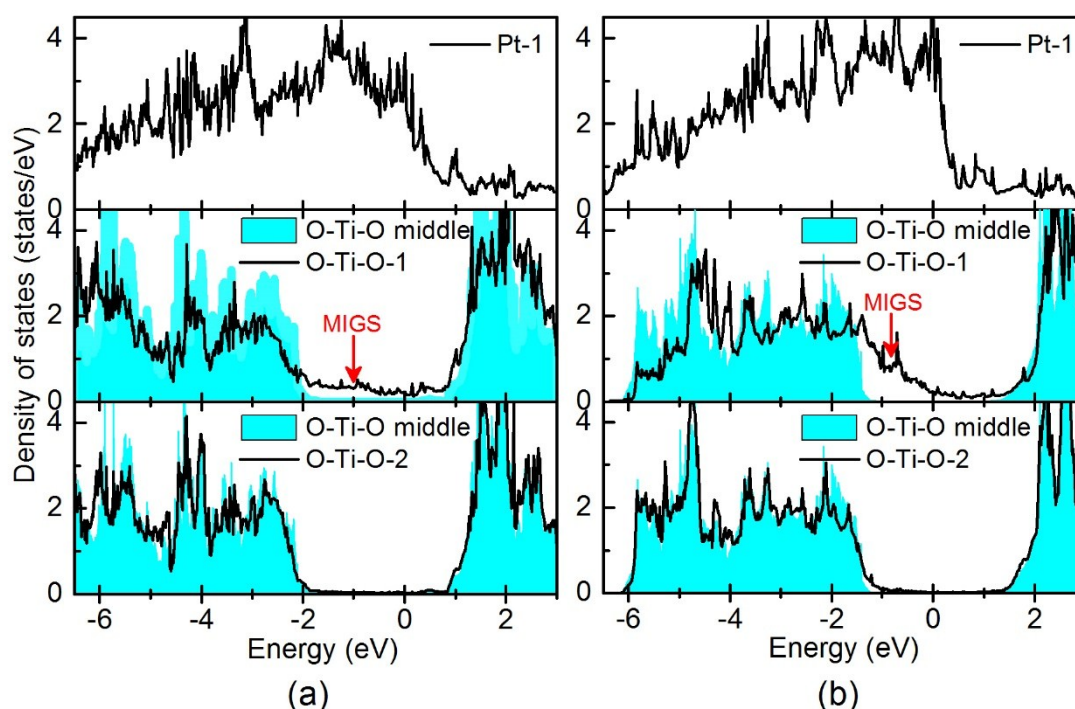


Figure S1. Layer-resolved density of states (LDOS) for the unstrained (a) interface A and (b) interface B. The shaded cyan regions represent the LDOS for the O-Ti-O atomic layer in the middle region of TiO₂ of the Pt/TiO₂ interface system. The Fermi level of Pt/TiO₂ interface system is set to 0 eV. The notation Pt/O-Ti-O-l refers to the l-th Pt/O-Ti-O atomic layer starting from the interface. MIGS denotes the so-called Metal-Induced Gap States.

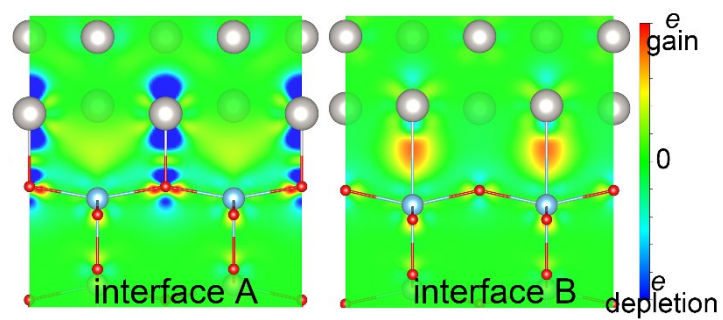


Figure S2. Calculated charge density differences for the unstrained Pt/TiO₂ (001) heterointerfaces.