Electronic supplementary information for "**Interface Schottky barrier engineering via strain in metal–semiconductor composite**"

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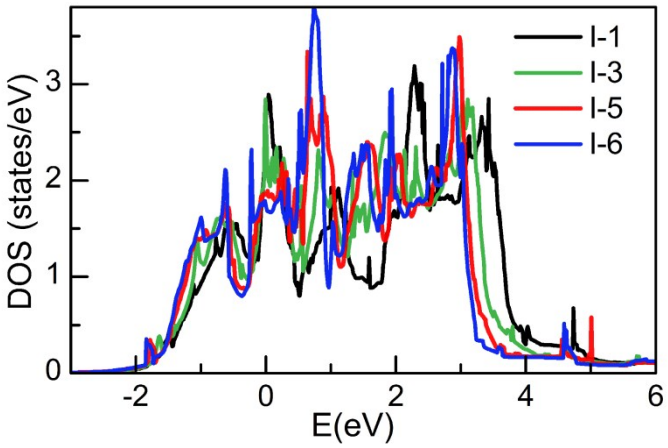

Figure S1. Density of states (DOS) of Au 5*d* states of Au in the same strained conditions as that in the I-1, I-3, I-5, and I-6 models, respectively. They are aligned by using their respective macroscopic average potentials as references.

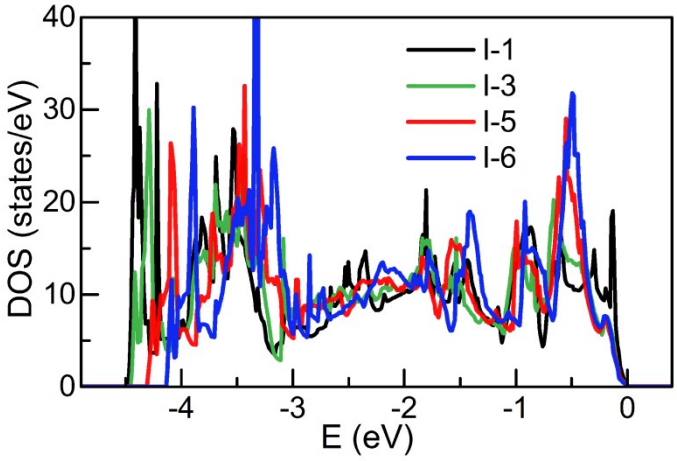

Figure S2. DOS for the valance bands of TiO_2 in the same strained conditions as that in the I-1, I-3, I-5, and I-6 interface models, respectively. The Fermi levels for the three strained TiO_2 are set at 0 eV.

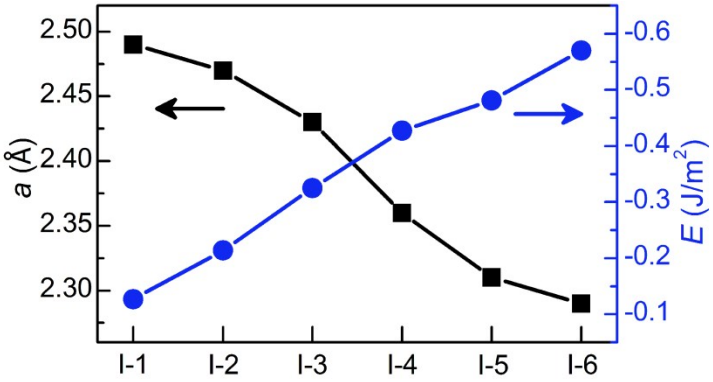

Figure S3. Interfacial Au–O_{2C} bond length *a* and interfacial energy *E* as a function of strain.

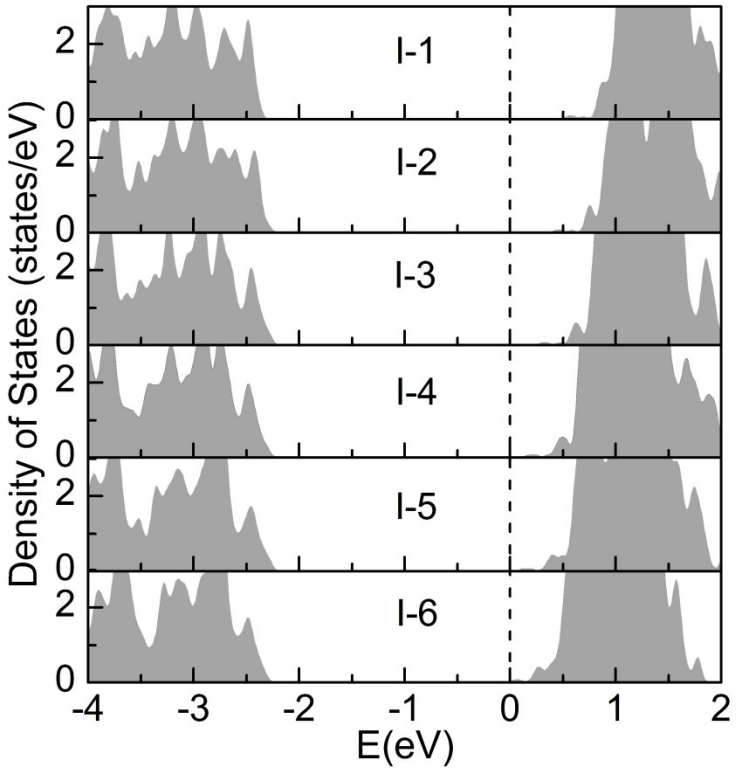

Figure S4. Local DOS for TiO_2 layers in the middle of the strained interfaces. The Fermi levels for all of the strained interfaces are set at 0 eV.

As shown in **Figure S4**, the Fermi level with respect to the VBM, which measures the Φ_p, only exhibits tiny change with strain; while the Fermi level with respect to the CBM measuring the Φ_n is significantly decreased. All of these are qualitatively in agreement with those obtained from the potential-line-up method.