Supplementary Information

Oxygen vacancy in Au/$SrTiO_3$ (001) interface: Stabilities, electronic properties and effect on photocatalysis

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Table S1. Calculated bulk Ov formation energy with different models. The same definition as that in Ref. [S1] is used for the bulk Ov formation energy.

Supercell	Lattice relaxation	Ov formation energy (eV)
2×2×2	unrelaxed	9.91
	relaxed	9.93
3×3×3	unrelaxed	9.81
	relaxed	9.82

Table S2. The determined SBHs from LDOS method for the examined interfaces with Ov.

Interface	IS1	IS2	IS3	IT1	IT2	IT3
SBH (eV)	0.2	0.1	-0.05	0.08	0.04	-0.02

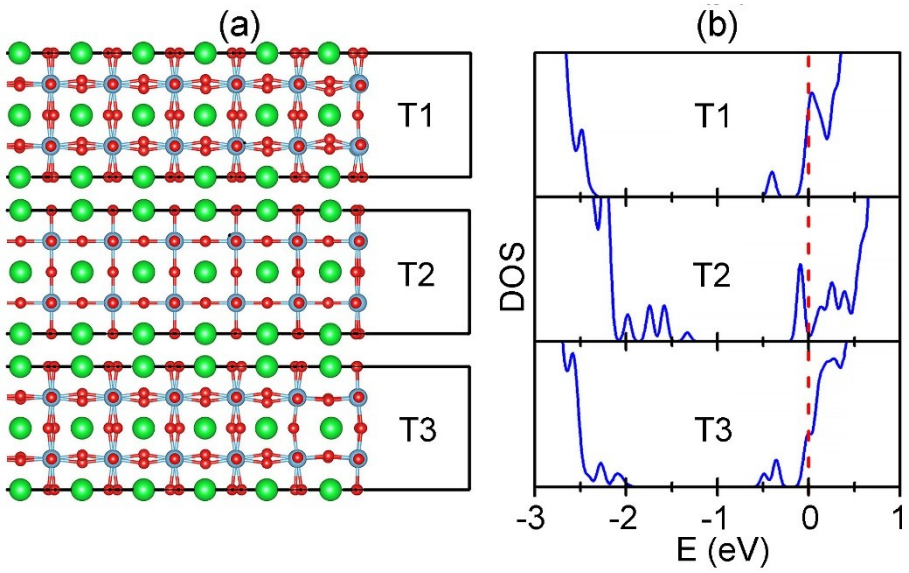

Figure S1. (a) Optimized geometric structures and (b) density of states (DOS) for the TiO_2 terminated surfaces with Ov in the T1, T2, and T3 atomic layers. The geometric structures and DOS for the other surfaces with Ov in the much inner SrO and TiO_2 layers are similar to the results for Ov in the T2 and T3 atomic layers, respectively. The dashed red line represents the Fermi level.

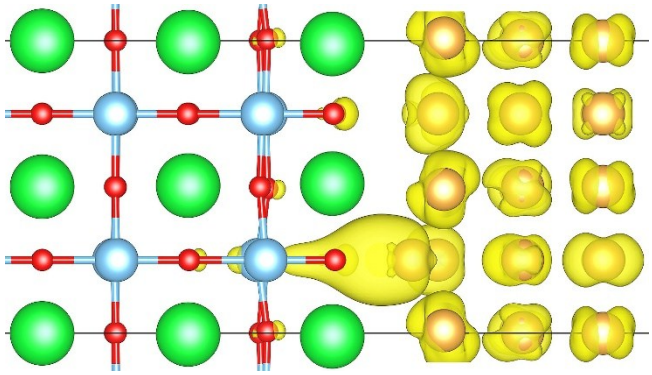

Figure S2. Three dimensional contour plot of the Ov introduced charge in the SrO terminated interface with Ov in the IS1 atomic layer. The isosurface value is at 0.001 e/Å^3.

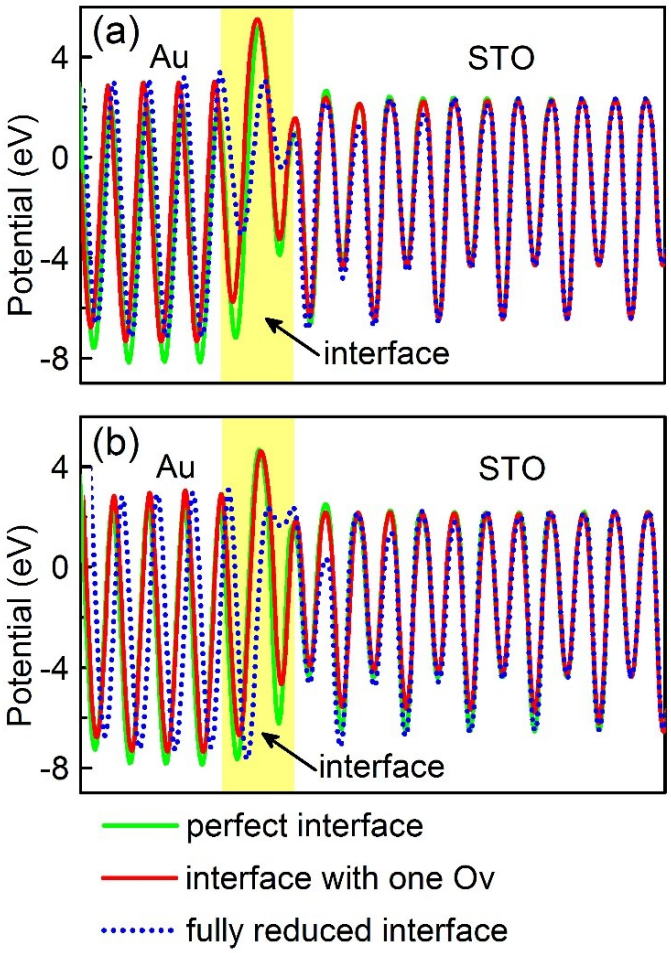

Figure S3. Local potentials for (a) SrO and (b) TiO_2 terminated Au/STO (001) interfaces. In (a) and (b), the three local potentials are aligned with each other by using their respective local potential in the STO bulk region as reference. In comparison to the system with perfect interface, the significantly increased local potentials of Au in the systems with one Ov at the interface and fully reduced interface demonstrates that the potential alignments between Au and STO are decreased.

References

[S1] V. E. Alexandrov, E. A. Kotomin, J. Maier and R. A. Evarestov, *Eur. Phys. J. B*, 2009, **72**, 53-57