Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

In Situ Exsolved Au Nanoparticles from Perovskite Oxide for Efficient Epoxidation of Styrene

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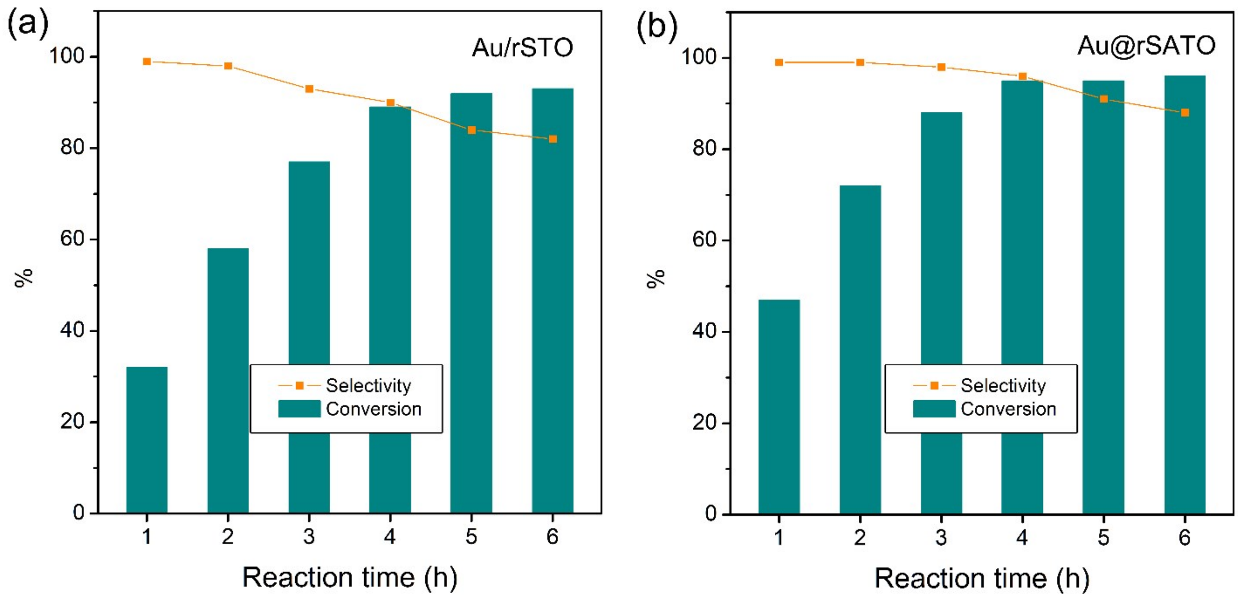

Figure S1. Conversion and selectivity of the *ex situ* deposited Au/rSTO and *in situ* exsolved Au@rSATO versus reaction time in 6h.

Table S1. Catalytic activity of supported AuNPs for styrene epoxidation.

Catalyst	Au wt. %	Oxidant	Conversion %	Selectivity %	Ref.
Au/STO	0.53	H_2O_2	65.2	91.7	This work
Au/rSTO	0.53	H_2O_2	88.5	90.1	This work
SATO	0.53	H_2O_2	21.6	96.4	This work
Au@rSATO	0.53	H_2O_2	95.0	96.3	This work
Au/MgO	7.5	TBHP	62.6	54.3	[1]
Au/Al_2O_3	6.36	TBHP	44	28	[2]
Au/TiO_2	6.0	TBHP	61	53	[3]
Au/Al_2O_3	2.0	TBHP	84.3	69.0	[4]
Au/LDH	0.66	TBHP	67.4	73.5	[5]
Au/BaTNT	1	TBHP	60.5	80.1	[6]
Au/Si	4	TBHP	98.5	82.8	[7]
Au/TS-1	1	H_2O_2	92.7	90.4	[8]
Au-2S-IL	4.5	H_2O_2	60.4	92.9	[9]

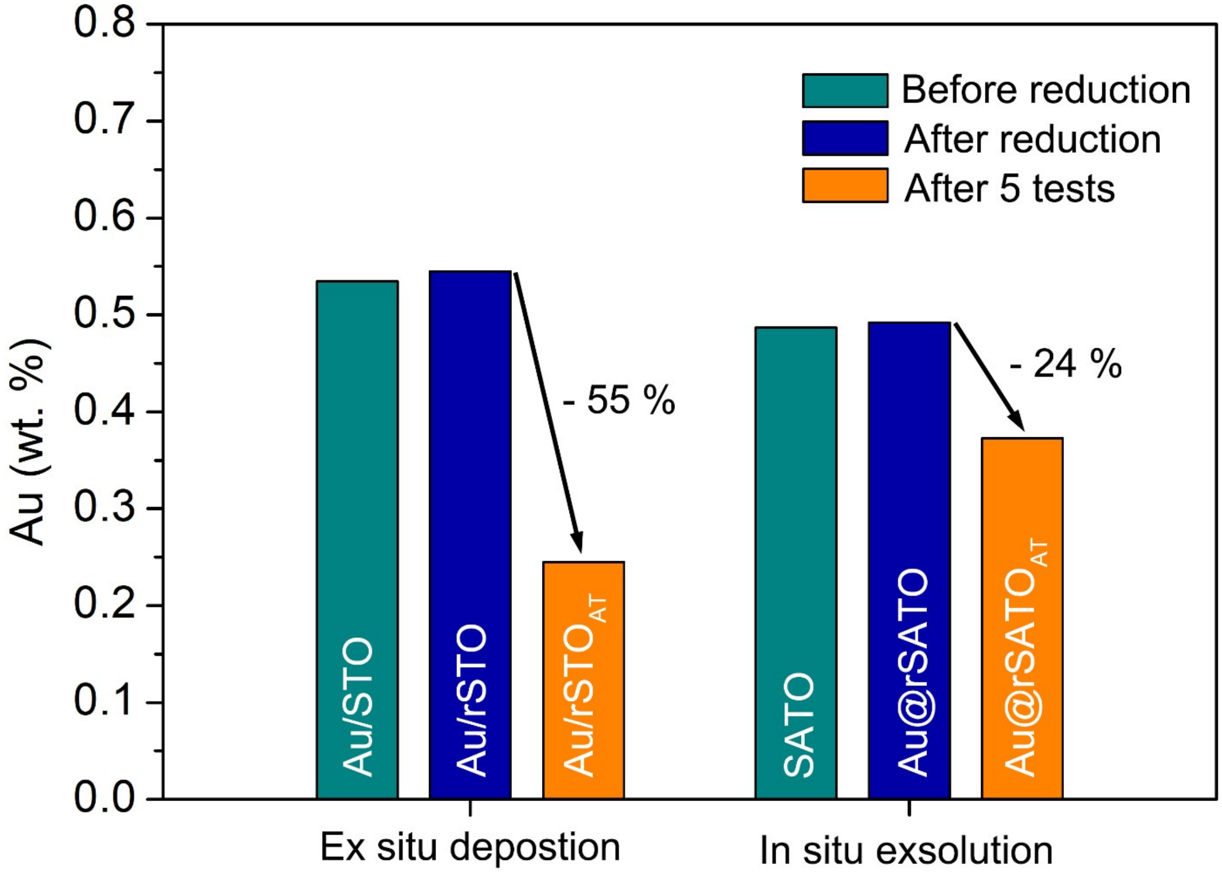

Figure S2. Weight ratio of Au in the as-prepared catalysts before and after catalysis obtained with ICP-OES.

Table S2. Elemental compositions of the as-prepared catalysts based on XPS analysis. The values show the relative atomic ratios of Sr and Au compared to Ti.

Elemental	Sr/Ti	Au/Ti
Au@rSATO	0.851	0.0055
SATO	0.806	0.0048
Au/rSTO	0.948	0.0050
Au/STO	0.915	0.0049
rSTO	0.953	/
STO	0.915	/

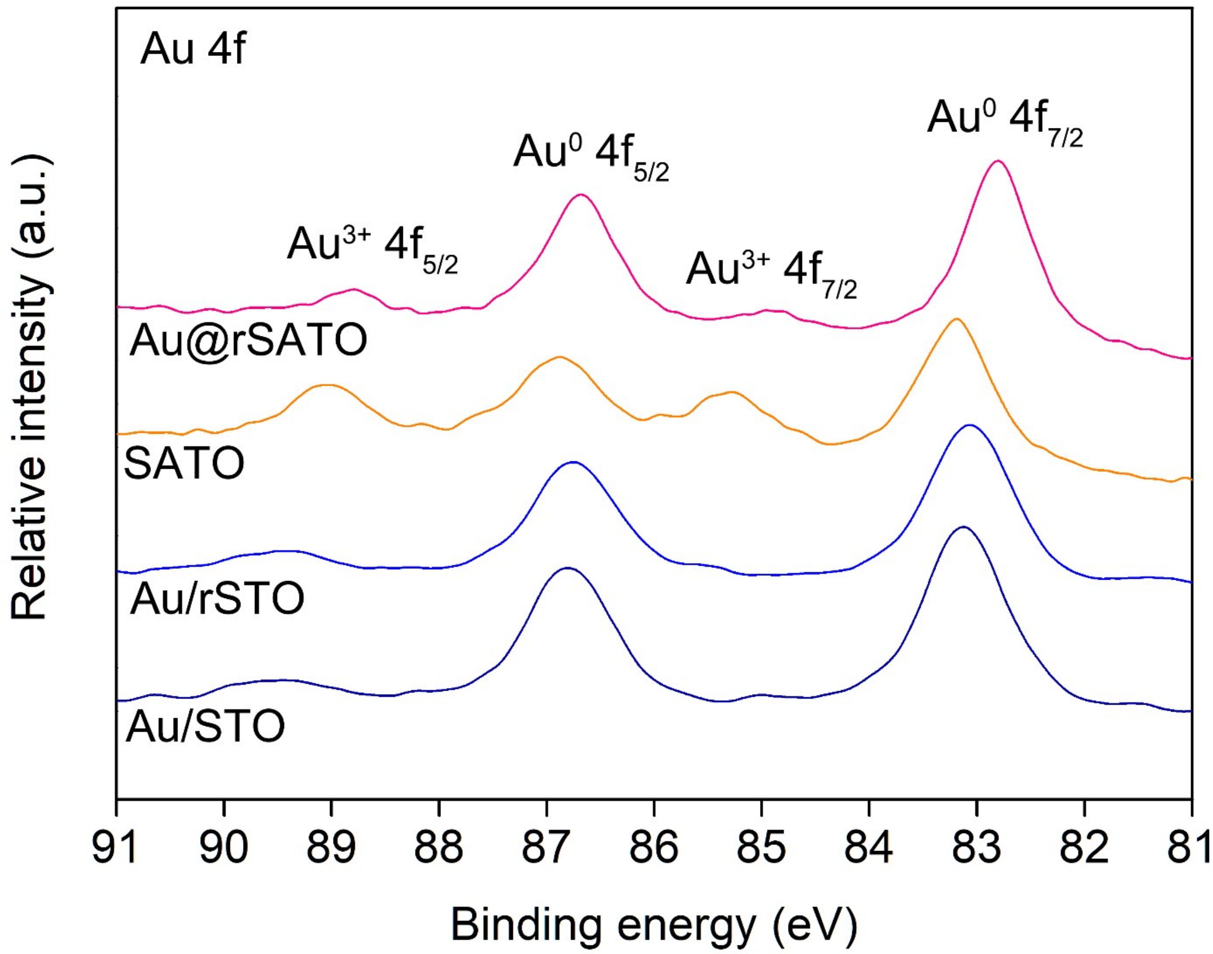

Figure S3. High-resolution Au spectra of the Au-containing samples.

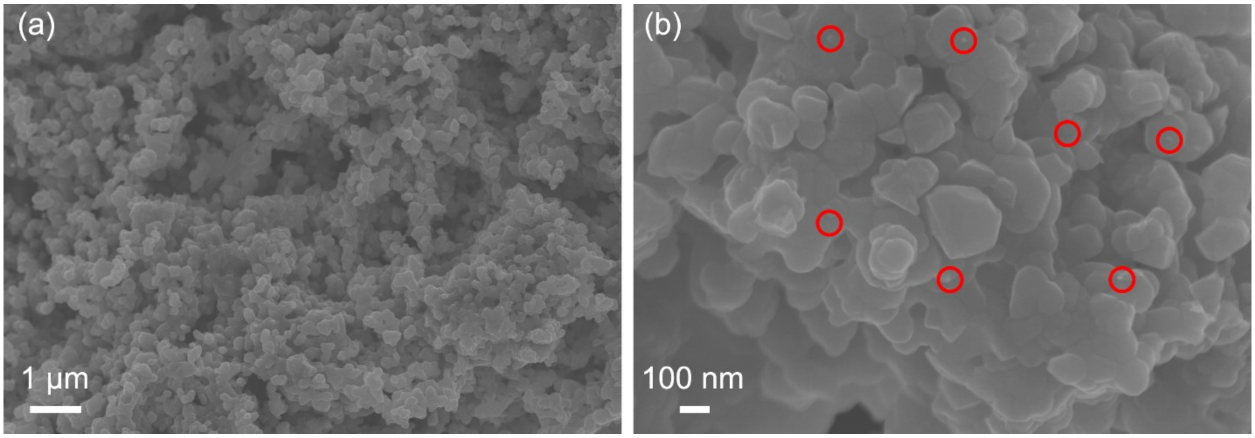

Figure S4. SEM images of Au@rSATO with different magnifications. The red circles highlight some of the exsolved nanoparticles.

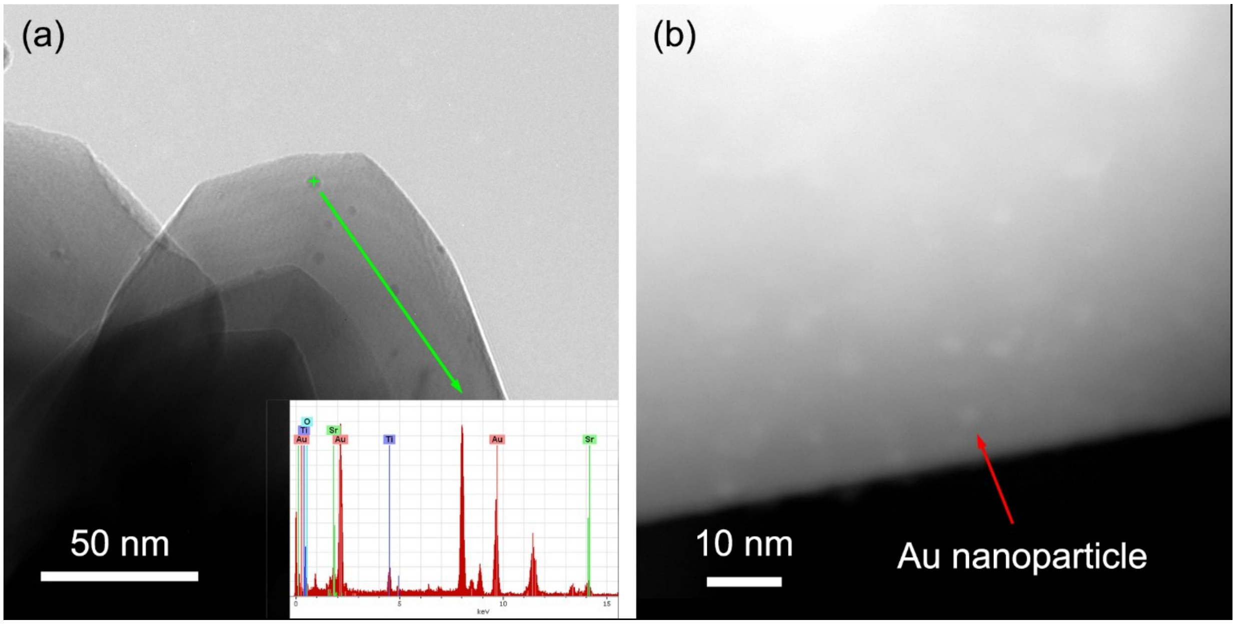

Figure S5. (a) EDX analysis of a selected Au nanoparticle for Au@rSATO. (b) HAADF-STEM image of Au@rSATO. Bright dots represent for the AuNPs.

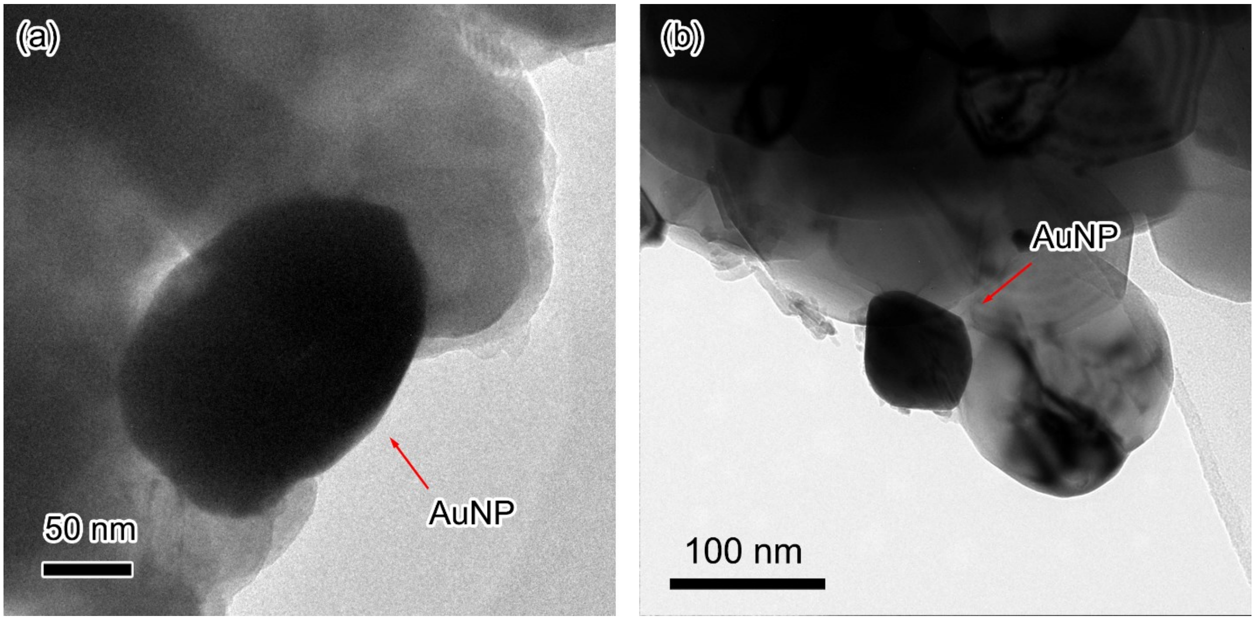

Figure S6. TEM images of the AuNPs in Au/rSTO.

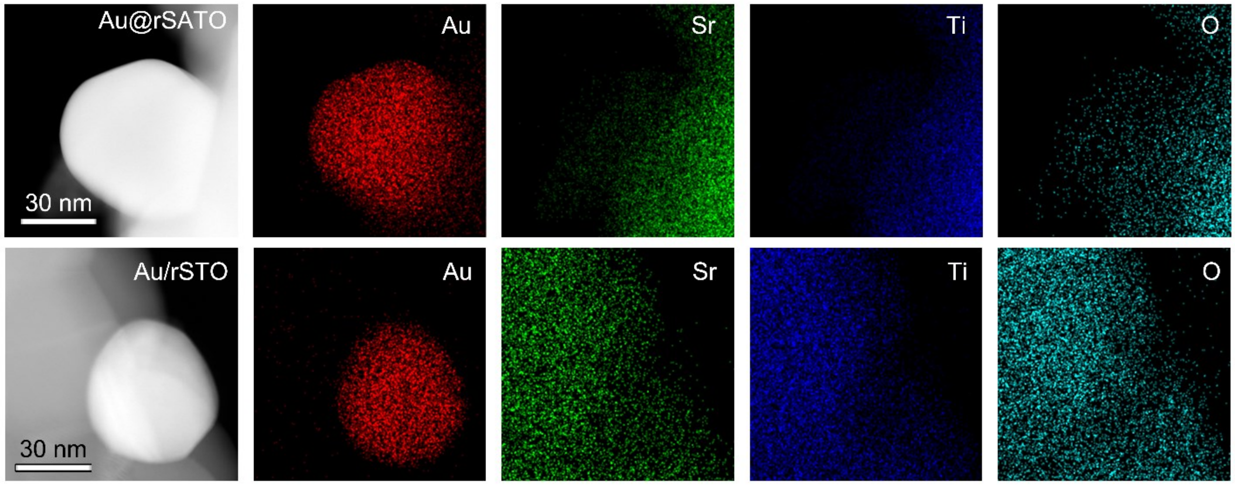

Figure S7. HAADF image and the corresponding EDX mappings of selected AuNPs for Au@rSATO (top) and Au/rSTO (bottom).

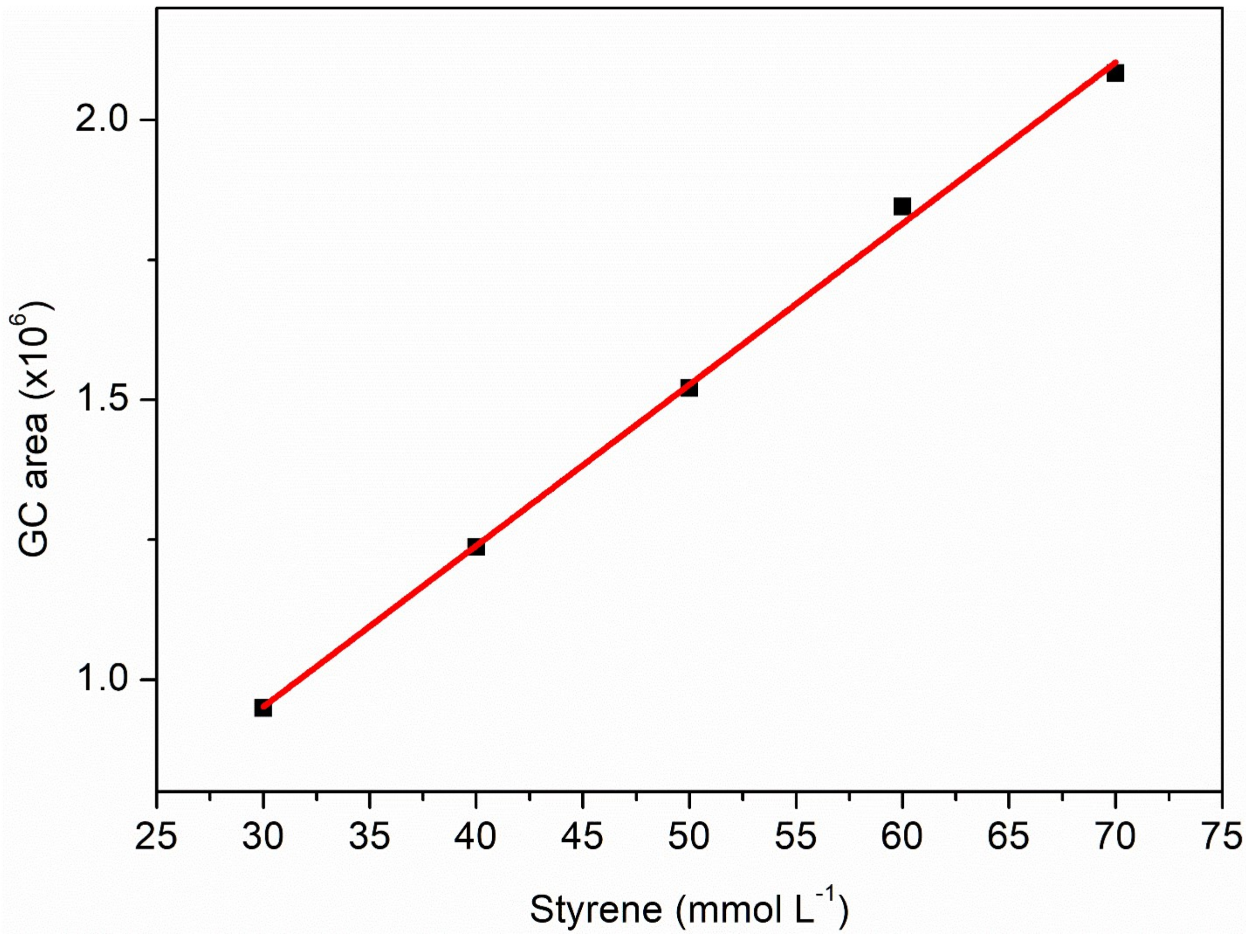

Figure S8. Calibration of the GC-area with standard styrene solutions of different concentrations (1 μL styrene solution with a split ratio of 1:50).

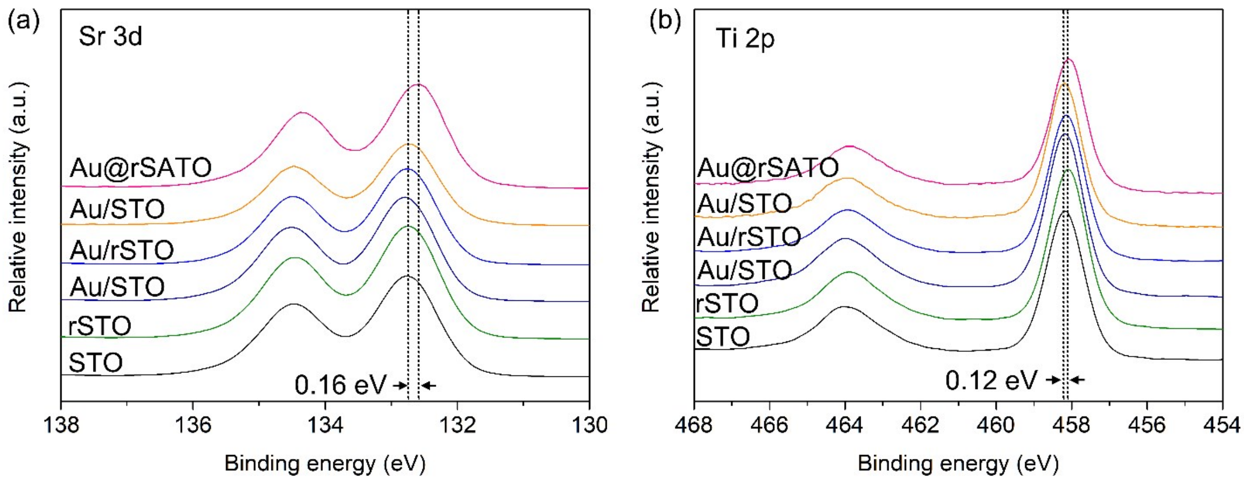

Figure S9. High-resolution Sr 3d and Ti 2p spectra of the as-prepared catalysts.

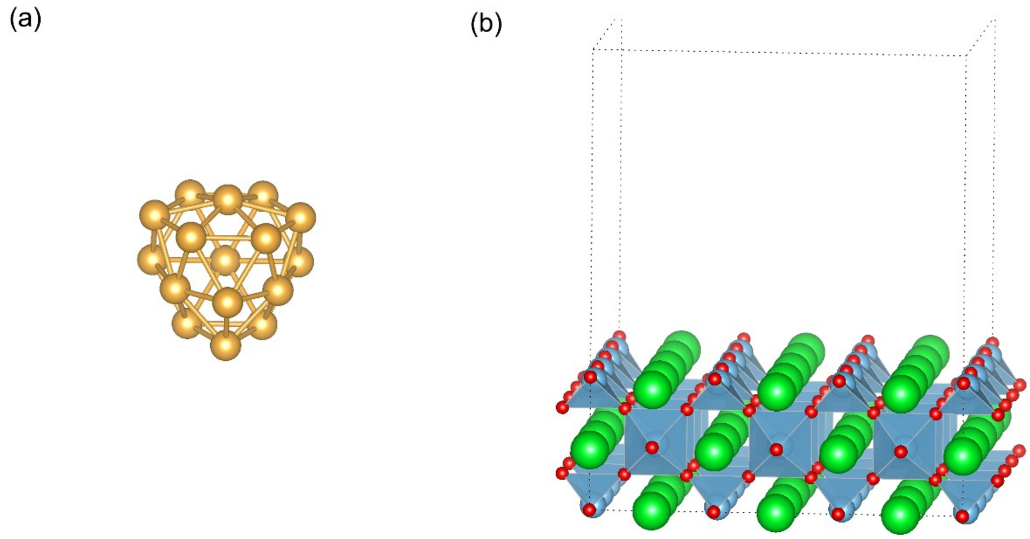

Figure S10. Relaxed slab models for (a) Au_{16} cluster, and (b) $SrTiO_3$ (110) surface with the bottom two layers are fixed.

Table S3.1. Coordinates and Bader charge of the Au atoms for Figure 6(f) in the main text.

Atom number	X	Y	Z	Charge (e^-)
1	13.707	6.905	7.912	0.498443
2	11.901	5.399	9.37	0.130842
3	7.672	5.399	9.352	0.129377
4	5.962	3.833	7.761	0.694315
5	7.704	8.282	9.51	0.070997
6	5.873	6.924	7.903	0.498174
7	13.607	3.831	7.761	0.70034
8	9.758	9.928	7.842	0.60733
9	9.783	6.636	10.566	0.028279
10	13.599	9.744	7.82	0.593205
11	9.779	6.997	7.76	0.484984
12	11.855	8.276	9.484	0.066647
13	9.788	9.575	10.645	0.182214
14	5.99	9.761	7.828	0.600224
15	9.793	4.148	7.955	0.439763
16	9.791	1.412	7.767	0.638329

Table S3.2. Coordinates and Bader charge of the Au atoms for Figure 6(g) in the main text.

Atom number	X	Y	Z	Charge (e^-)
1	9.523	9.159	7.638	0.035284
2	6.467	9.099	12.194	-0.02098
3	8.757	10.498	12.092	0.019555
4	5.635	7.692	9.953	0.013918
5	7.684	5.828	9.726	-0.09355
6	8.821	5.02	12.176	0.021363
7	7.648	9.661	9.686	-0.09514
8	10.35	5.048	9.873	0.021877
9	7.142	7.757	7.729	0.01242
10	11.182	6.461	12.11	-0.02293
11	9.558	6.395	7.689	0.00954
12	10.323	10.529	9.812	0.02386
13	10.983	7.794	9.623	-0.0949
14	11.182	9.145	12.046	0.048927
15	6.473	6.337	12.216	0.054393
16	8.829	7.765	12.802	-0.08855

Table S3.3. Coordinates and Bader charge of the Au atoms for Figure 6(h) in the main text.

Atom number	**X**	**Y**	**Z**	**Charge (e^-)**
1	5.513	6.809	12.307	0.037373
2	10.226	9.615	12.35	0.079694
3	7.848	8.225	12.999	-0.032404
4	8.754	6.942	7.892	0.33344
5	10.223	6.931	12.367	0.05145
6	10.111	8.306	9.899	-0.017959
7	9.446	11.038	10.112	0.132677
8	8.722	9.707	7.888	0.27777
9	7.801	10.97	12.335	0.08216
10	5.509	9.571	12.333	0.086698
11	6.81	6.342	9.852	0.055361
12	4.755	8.204	10.04	0.129941
13	6.776	10.175	9.877	0.058941
14	7.861	5.49	12.326	0.079822
15	6.338	8.306	7.872	0.570837
16	9.469	5.557	10.079	0.132963

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