Identification of the Catalytic Site at the Interface Perimeter of Au Clusters on Rutile TiO_2(110)
Supplemental Material

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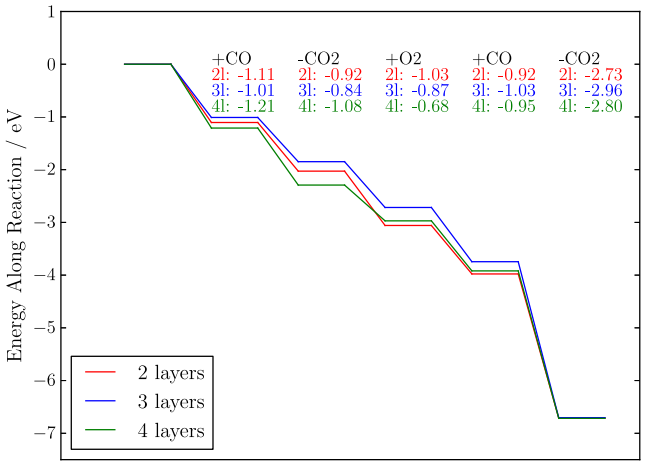

Figure S1. Comparison of reaction energetics calculated with a 2 tri-layer, 3 tri-layer and 4 tri-layer TiO_2(110) slab. The reaction energetics are for the reaction shown in Fig. 5 of the main text.

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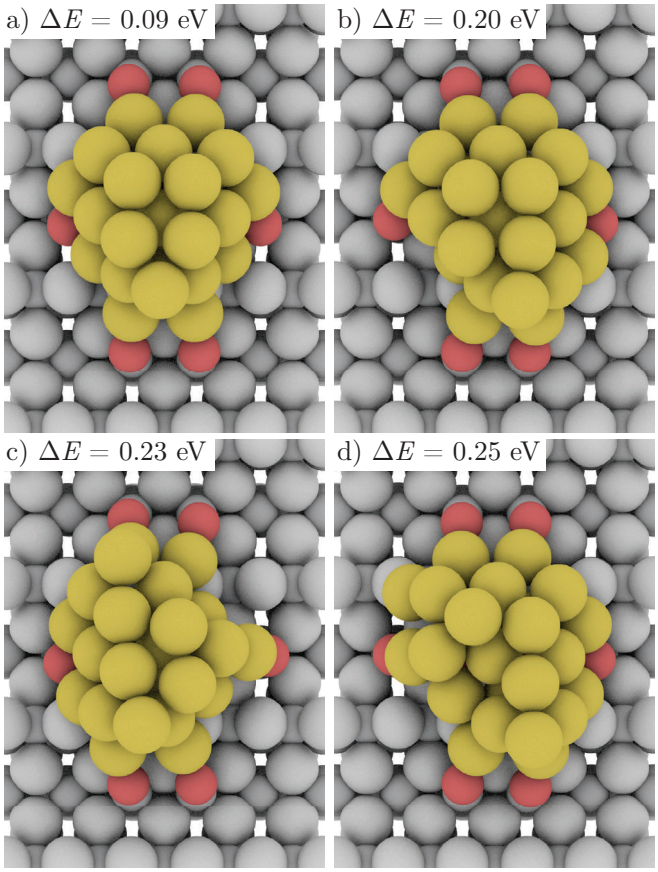

Figure S2. A selection of low energy isomers of the Au_{24} cluster adsorbed on the TiO_2(110) surface prepatterned with 8 O atoms. The energy difference at each structure is relative to the most stable isomer shown in Fig. 1b of the main text.

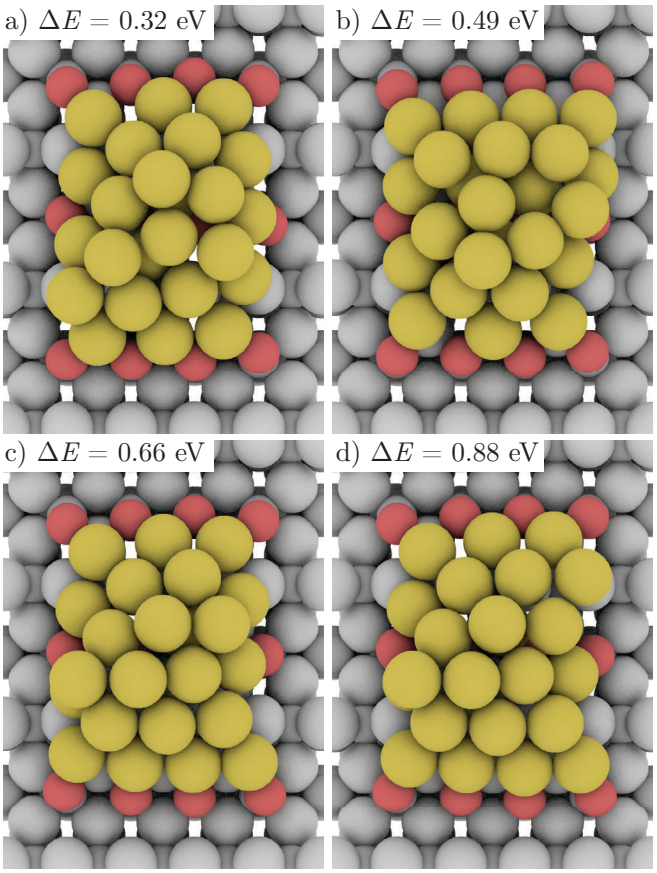

Figure S3. A selection of low energy isomers of the Au_{24} cluster adsorbed on the TiO_2(110) surface prepatterned with 12 O atoms. The energy difference at each structure is relative to the most stable isomer shown in Fig. 1c of the main text.

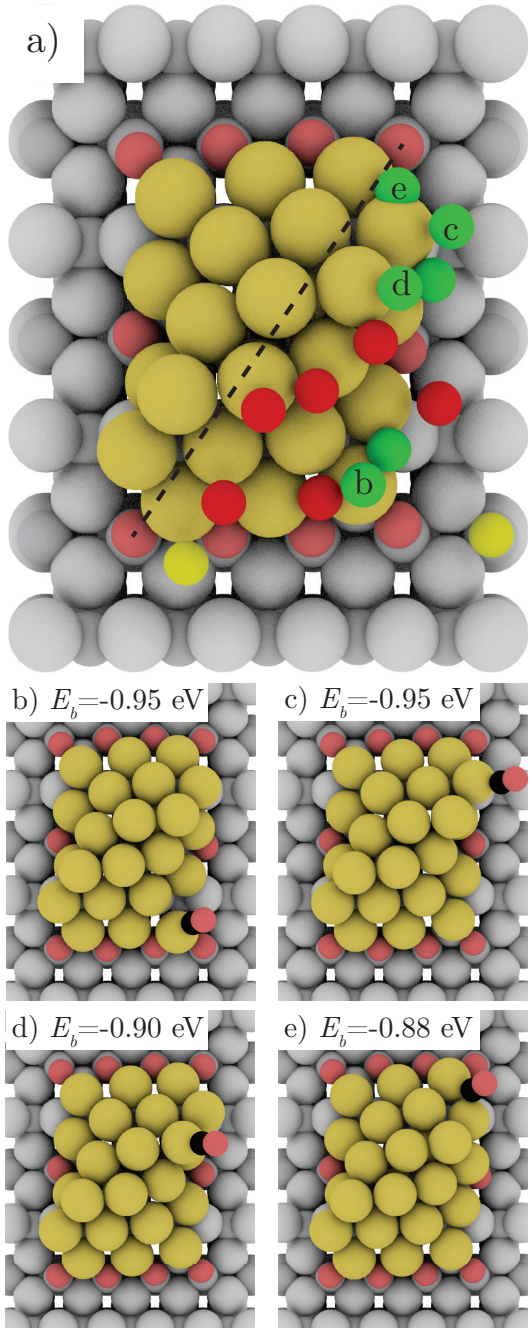

Figure S4. a) shows the position of the C atom for all tested CO adsorption sites. Yellow spheres mark CO adsorption sites with an adsorption energy similar to CO in the trough. Red spheres weaker and green spheres stronger adsorption sites. The two green spheres not annotated in image a are shown in Fig. 2 of the letter with the others shown in image b to e here.

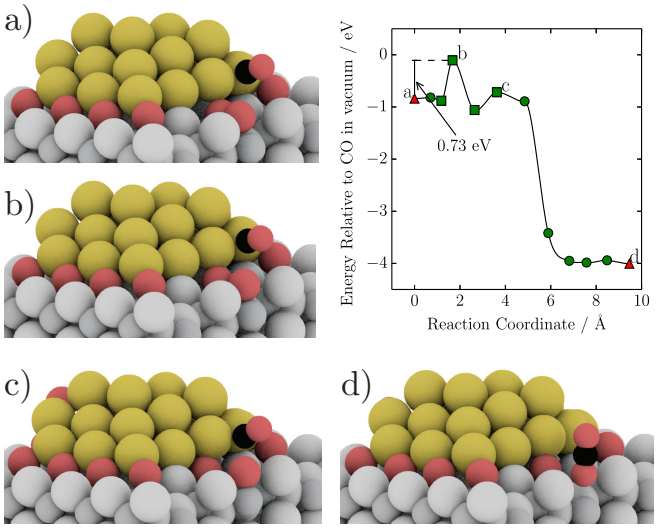

Figure S5. The reaction from image e to a in Fig. 4. Red triangles are local minima, green circles are from NEB calculations, and green squares from CI-NEB calculations.

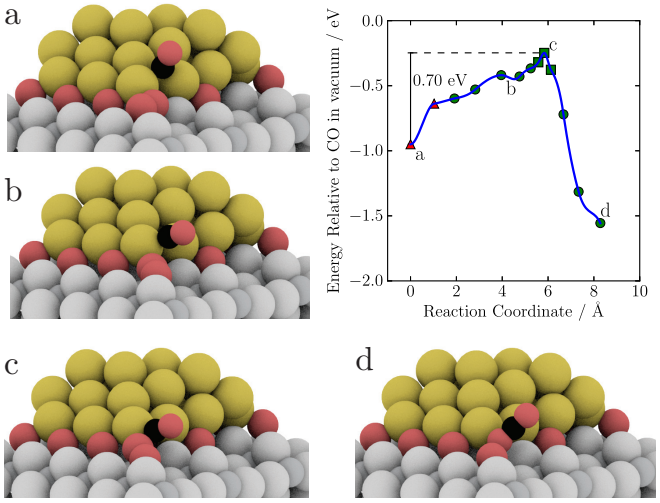

Figure S6. The reaction from image e to a in Fig. 5. Red triangles are local minima, green circles are from NEB calculations, and green squares from CI-NEB calculations.

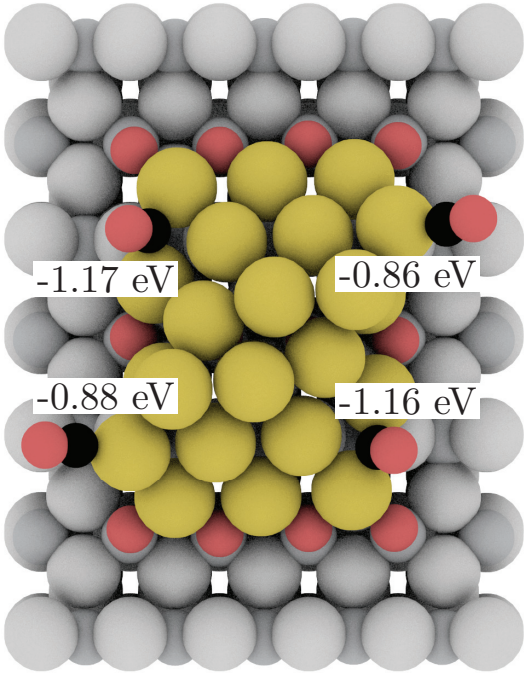

Figure S7. CO adsorbed at each corner of the Au_{24} cluster. The adsorption sites used in the lower right and upper left corner are the ones from Fig. 2c and the other two sites the ones from Fig. S4c. The four adsorption energies quoted in the figure are calculated as differential binding energies i.e. minus the energy cost of removing that particular CO leaving the other three behind. Comparing these differential adsorption energies it is seen that CO binds with between 0.04 eV and 0.09 eV less when several CO molecules adsorb simultaneously.