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Supporting Information for

Understanding the Enhanced Catalytic Activity of the Bimetallic AuCu/TiO_2 in CO_2 Adsorption and Activation: A Density Functional Theory Study

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Table S1. The Mulliken Charges Carried by Au Atom on the $Au_{10}/TiO_2(101)$ Surface, Calculated at the GGA+U Level, with U=3.5 eV

$Au_{10}/TiO_2(101)$	Au1	Au2	Au3	Au4	Au5	Au 6	Au 7	Au8	Au 9	Au10	Total
Charge/|e|	-0.11	0.00	-0.13	-0.10	-0.11	-0.03	-0.07	-0.14	0.04	-0.15	-0.80

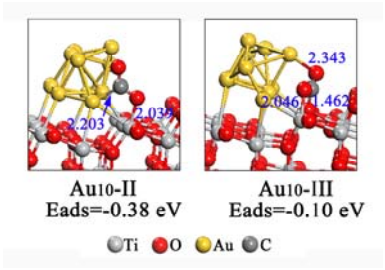

Figure S1. CO_2 adsorption configurations selected for testing on $Au_{10}/TiO_2(101)$ surface. Calculated at the GGA+U level, with U=3.5 eV.

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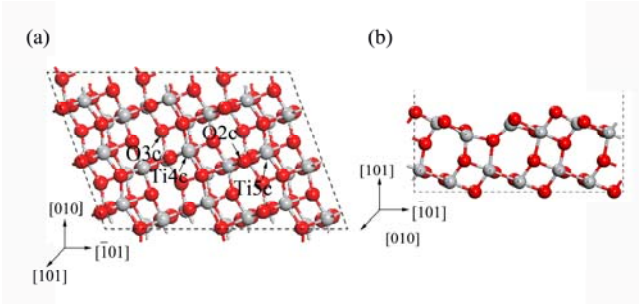

Figure S2. Top (a) and side (b) views of the defective TiO_2(101) surface.

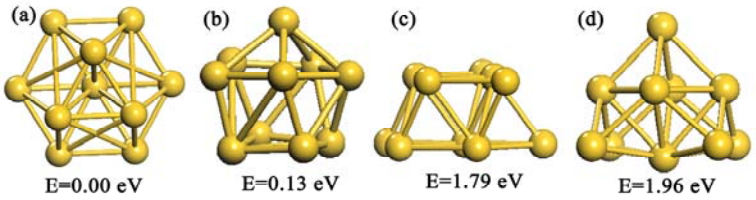

Figure S3. The structures of the Au_{10} cluster.

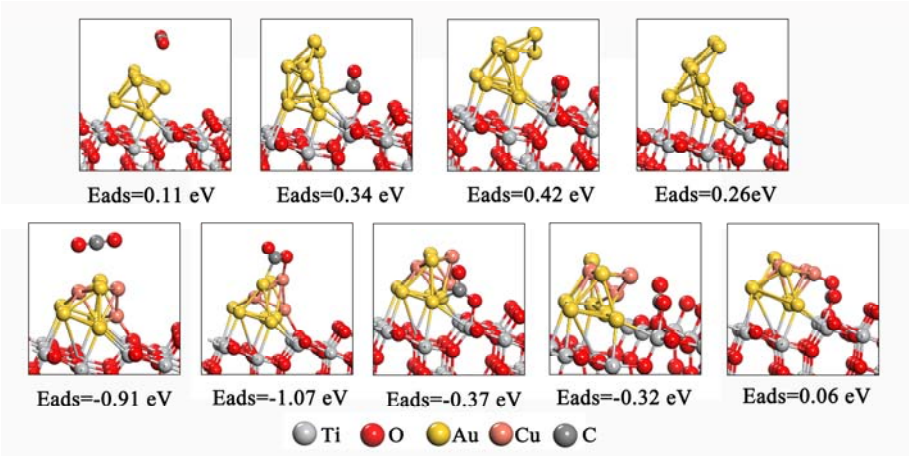

Figure S4. Optimized less stable binding configurations of CO_2 adsorbed on Au_{10}/TiO_2(101) and Au_7Cu_3/TiO_2(101) surfaces.

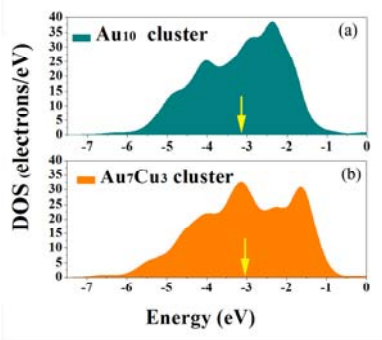

Figure S5. The pDOS of the Au_{10} and Au_7Cu_3 clusters on TiO_2(101) surface. The d-band center is marked by yellow arrow. The Fermi level is set to 0 eV.