Supporting Information for

Adsorption and Reaction of C_2H_4 and O_2 on Nano-sized Gold Cluster: A Computational Study

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Table S1. Calculated Adsorption Energies (in eV), Geometrical Parameters (Å) of Weakly Adsorbed C_2H_4 on Au_{38} Nanocluster.

Table S2. Calculated Adsorption Energies (in eV), Geometrical Parameters (Å) of Weakly Adsorbed O_2 on Au_{38} Nanocluster.

Figure S1. The calculated weakly bound intermediates of C_2H_4 adsorbed on Au_{38} nanocluster.

Figure S2. The calculated weakly bound intermediates of O_2 adsorbed on Au_{38} nanocluster.

Figure S3. The calculated electronic local density of states (LDOS) of the system projected on the orbitals for the adsorbed constructs of O_2 (left panel) and C_2H_4 (right panel) species, as well as the *d*-projected of the Au atoms on the hexagonal fcc(111)-like face. O_a and O_g represent the remaining oxygen atom adsorbed on the nanocluster and the oxygen atom of epoxide or acetaldehyde.

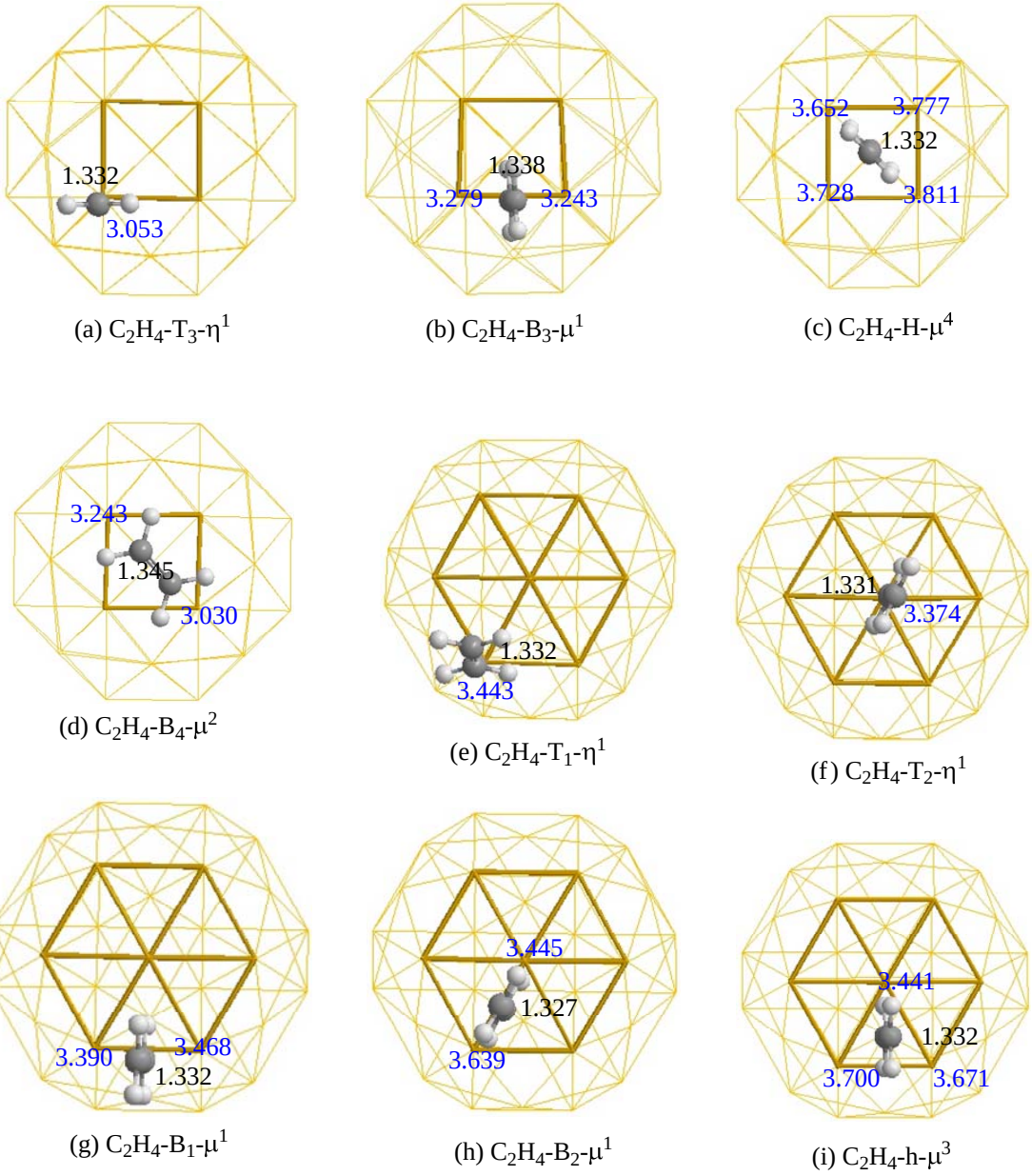
Figure S4. The electronic local density of states (LDOS) of the system projected on the *d*-states of the Au38 nanoparticle and Au (111) surface.

Table S1. Calculated Adsorption Energies (in eV), Geometrical Parameters (Å) of Weakly Adsorbed C_2H_4 on Au_{38} Nanocluster.

species	E_{ads}(eV)	d_{Au1-C1}(Å)	d_{C1-C2}(Å)	d_{C2-Au2}(Å)
C_2H_4-T_3-η^1	0.05	3.053	1.332	
C_2H_4-B_3-μ^1	0.05	3.279	1.338	3.243
C_2H_4-H-μ^4	0.02	3.811, 3.728, 3.652, 3.777	1.332	
C_2H_4-B_4-μ^2	-0.04	3.243	1.345	3.030
C_2H_4-T_1-η^1	-0.15	3.443	1.332	
C_2H_4-T_2-η^1	-0.12	3.374	1.331	
C_2H_4-B_1-μ^1	0.01	3.390, 3.468	1.332	
C_2H_4-B_2-μ^1	-0.11	3.639, 3.445	1.327	
C_2H_4-h-μ^3	-0.04	3.441, 3.700, 3.671	1.332	

Table S2. Calculated Adsorption Energies (in eV), Geometrical Parameters (Å) of Weakly Adsorbed O_2 on Au_{38} Nanocluster.

O_2 species	E_{ads}(eV)	d_{Au1-O1}(Å)	d_{O1-O2}(Å)	d_{O2-Au2}(Å)
O_2-T_1-η^1-2	-0.09	2.154	1.294	
O_2-T_2-η^1	0.24	2.258	1.287	
O_2-T_1-η^2	0.16	2.315	1.359	2.270
O_2-T_2-η^2	0.06	2.491	1.309	2.404
O_2-h-μ^3	-0.09	2.385, 2.378, 2.484	1.311	

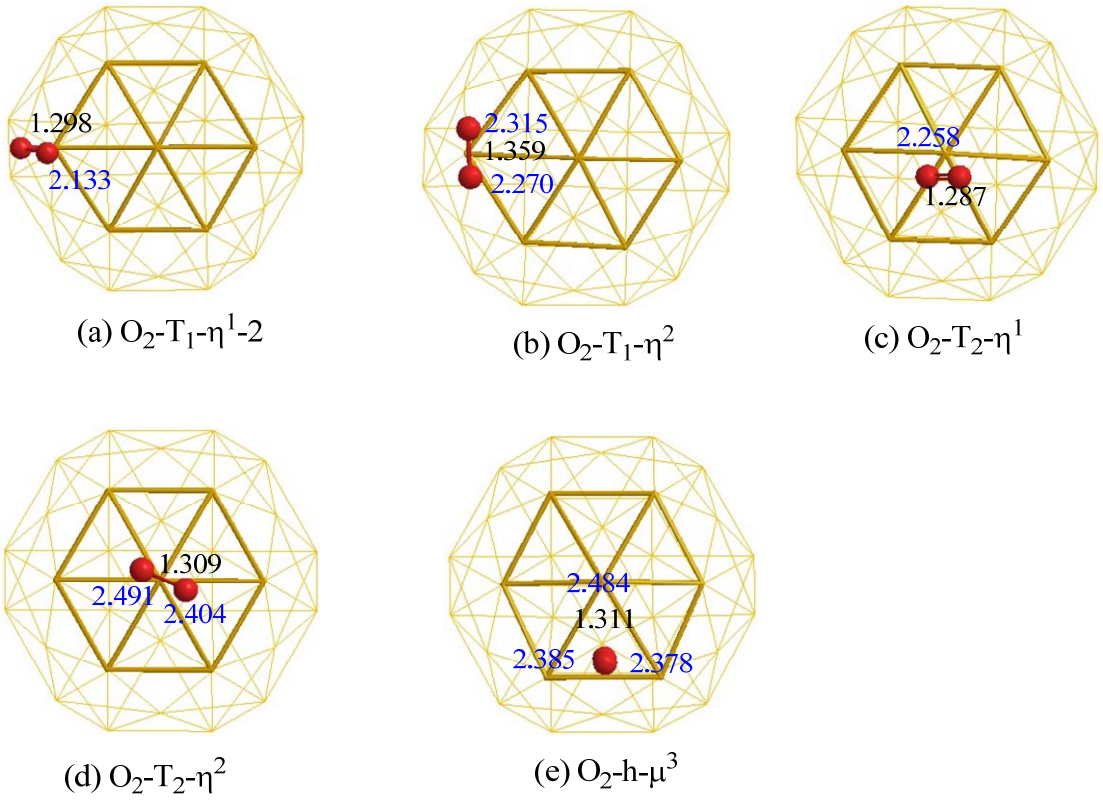


(a) C_2H_4-T_3-η^1 (b) C_2H_4-B_3-μ^1 (c) C_2H_4-H-μ^4

(d) C_2H_4-B_4-μ^2 (e) C_2H_4-T_1-η^1 (f) C_2H_4-T_2-η^1

(g) C_2H_4-B_1-μ^1 (h) C_2H_4-B_2-μ^1 (i) C_2H_4-h-μ^3

Figure S1. The calculated weakly bound intermediates of C_2H_4 adsorbed on Au_{38} nanocluster.



(a) O_2-T_1-η^1-2 (b) O_2-T_1-η^2 (c) O_2-T_2-η^1

(d) O_2-T_2-η^2 (e) O_2-h-μ^3

Figure S2. The calculated weakly bound intermediates of O_2 adsorbed on Au_{38} nanocluster.

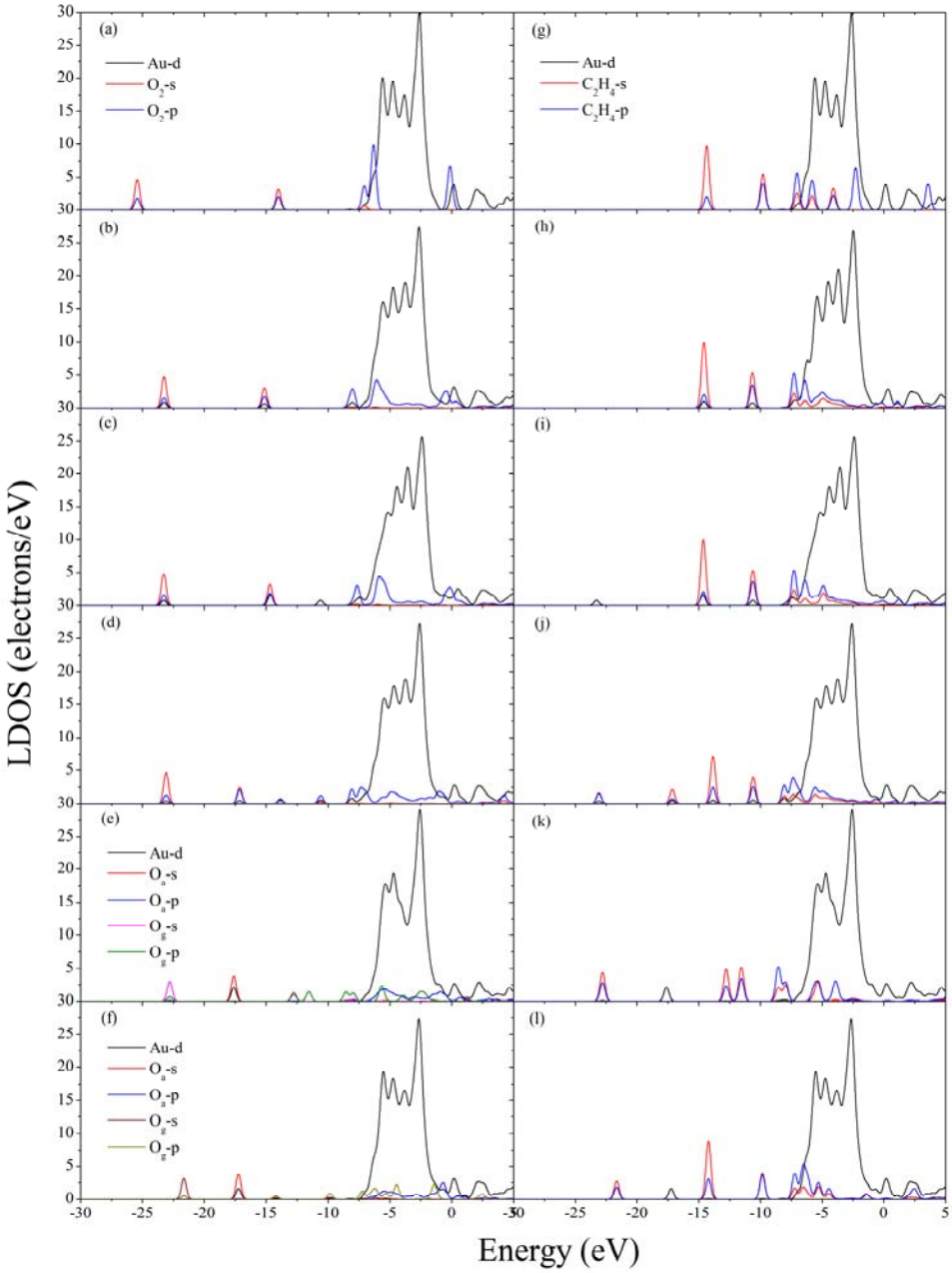


Figure S3. The calculated electronic local density of states (LDOS) of the system projected on the orbitals for the adsorbed constructs of O_2 (left panel) and C_2H_4 (right panel) species, as well as the *d*-projected of the Au atoms on the hexagonal fcc(111)-like face. O_a and O_g represent the remaining oxygen atom adsorbed on the nanocluster and the oxygen atom of epoxide or acetaldehyde.

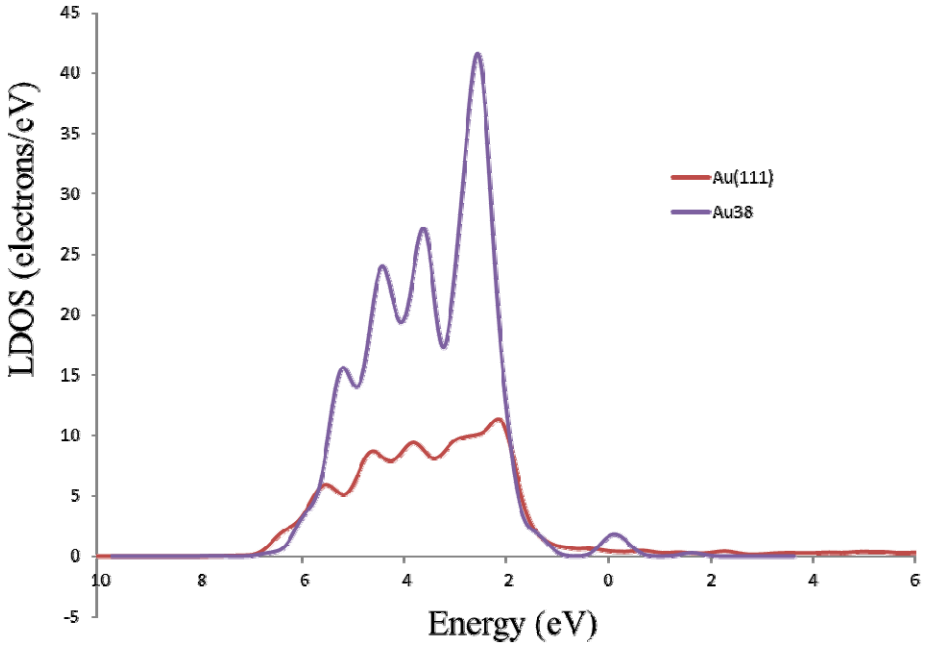


Figure S4. The electronic local density of states (LDOS) of the system projected on the *d*-states of the Au_{38} nanoparticle and Au (111) surface.