Supporting Information

A Water-Promoted Mechanism of Alcohol Oxidation on Au(111) Surface: Understanding toward the Catalytic Behavior of Bulk Gold

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Table S1. Calculated Adsorption Energy (E_{ad}) of the Key Species on Au(111) Surface Using Different *k*-points

Species	E_{ad} (3×3×1) / eV [a]	E_{ad} (7×7×1) / eV [b]	$\|E_{ad}\|$ / eV [c]
CH_3OH	–0.17	–0.16	0.01
CH_3O	–0.79	–0.87	0.08
CH_2O	–0.06	–0.06	0.00
O	–2.64	–2.73	0.09
OH	–1.54	–1.61	0.07
OOH	–0.24	–0.30	0.06

[a] Adsorption energy obtained using 3×3×1 k-point. [b] Adsorption energy obtained using 7×7×1 k-point. [c] The difference between E_{ad} (3×3×1) and E_{ad} (7×7×1), in absolute value.

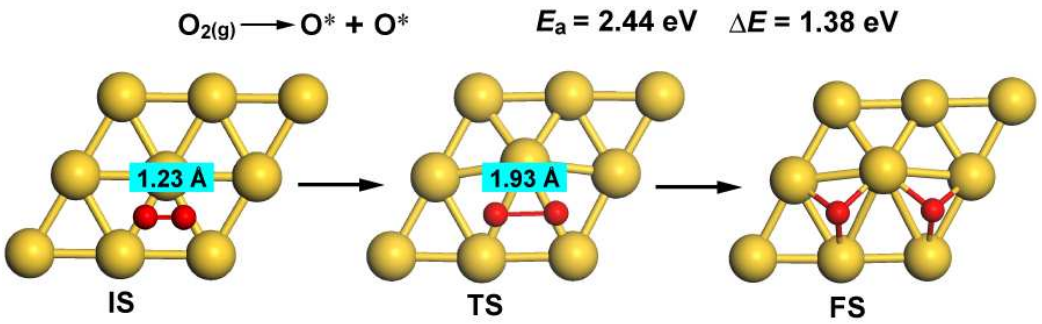

Figure S1. The dissociation of molecular oxygen on Au(111) surface.

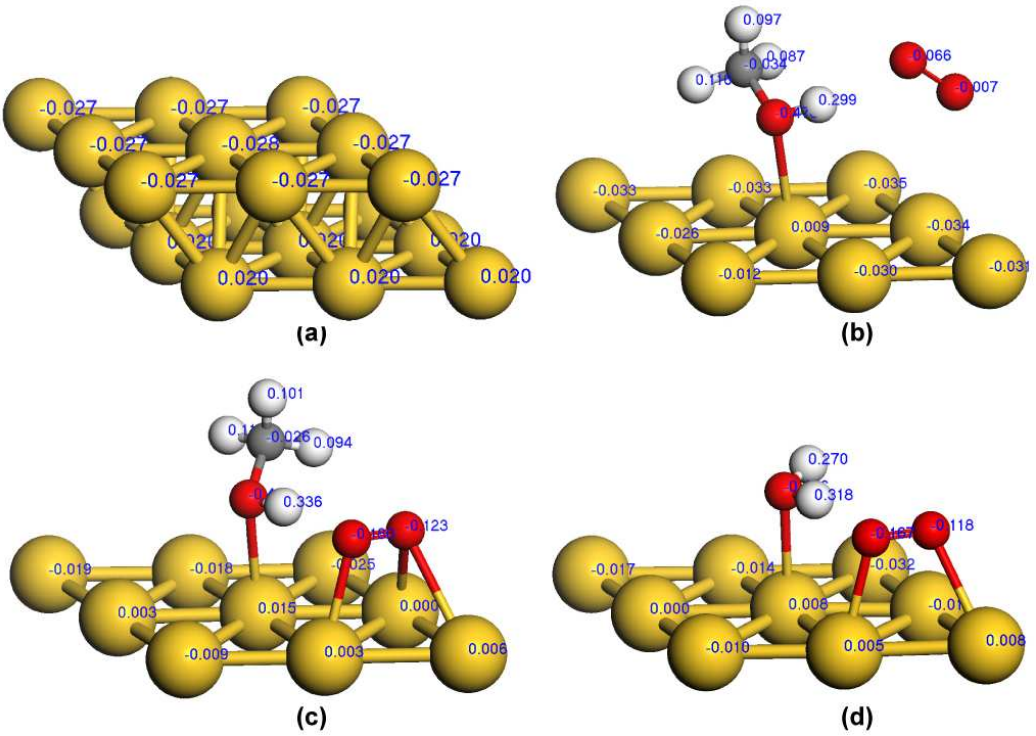

Figure S2. Mulliken charge distribution on selected models. (a) top-two layers of Au(111) surface. (b) adsorbed CH_3OH and gas phasO_2. (c) co-adsorbed CH_3OH and O_2. (d) co-adsorbed H_2O and O_2.

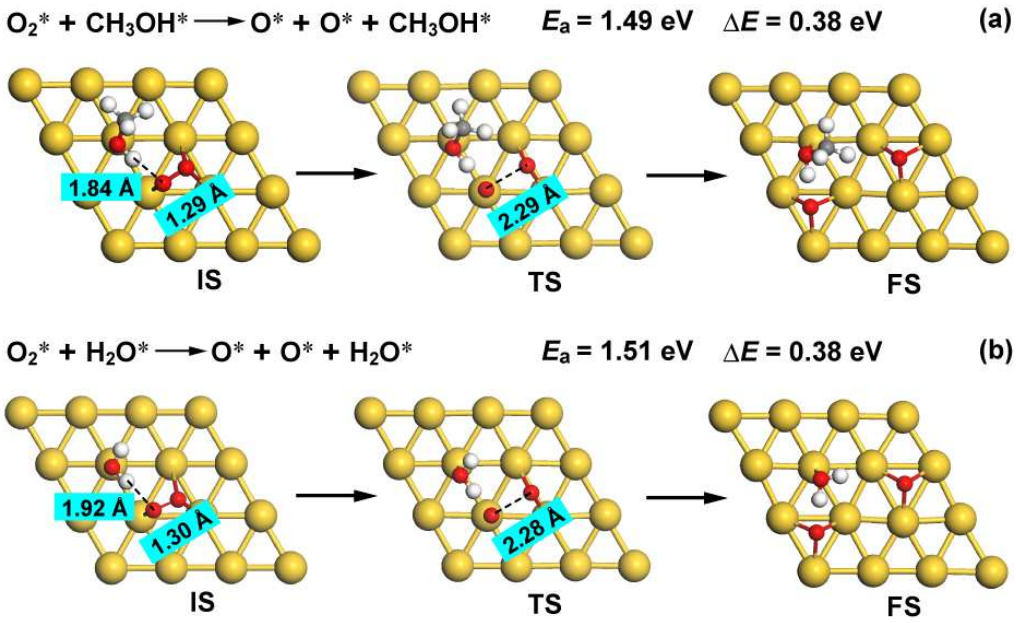

Figure S3. The dissociation of molecular oxygen in the presence of neighboring CH_3OH (a) and H_2O (b)on Au(111) surface.

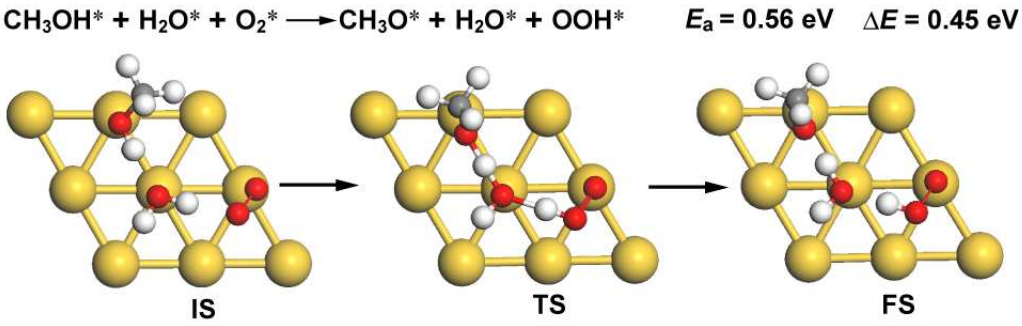

Figure S4. The formation of OOH with a H_2O molecule locating in the middle of CH_3OH and O_2.

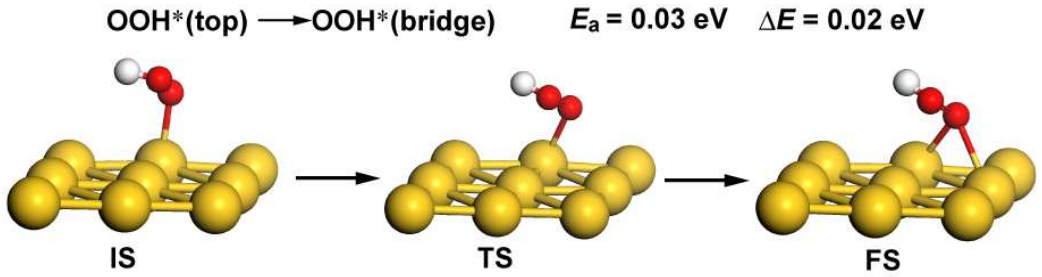

Figure S5. The diffusion of OOH* from top to bridge site on Au(111) surface.

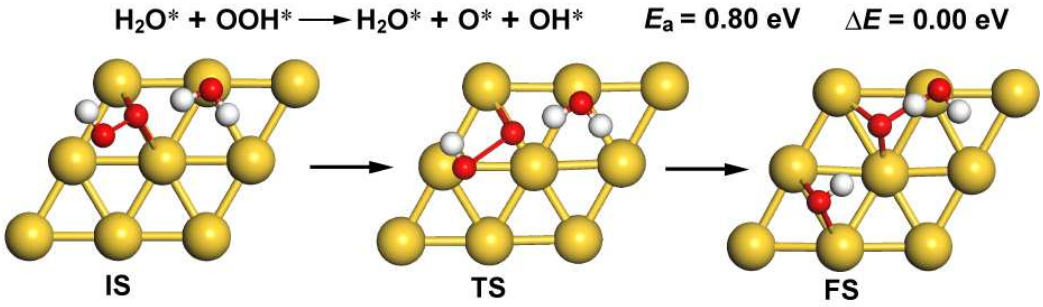

Figure S6. The dissociation of *OOH in the presence of neighboring H_2O on Au(111) surface.

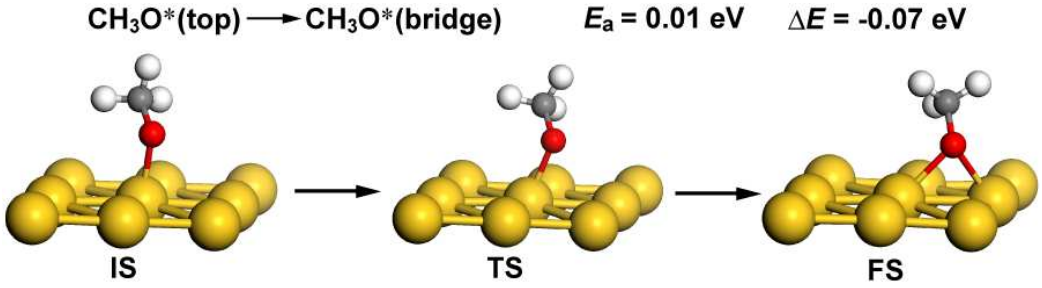

Figure S7. The diffusion of CH_3O^* from top to bridge site on Au(111) surface.