Supporting information

Insights into reaction mechanisms of ethanol electrooxidation at the Pt/Au(111) interfaces by density functional theory

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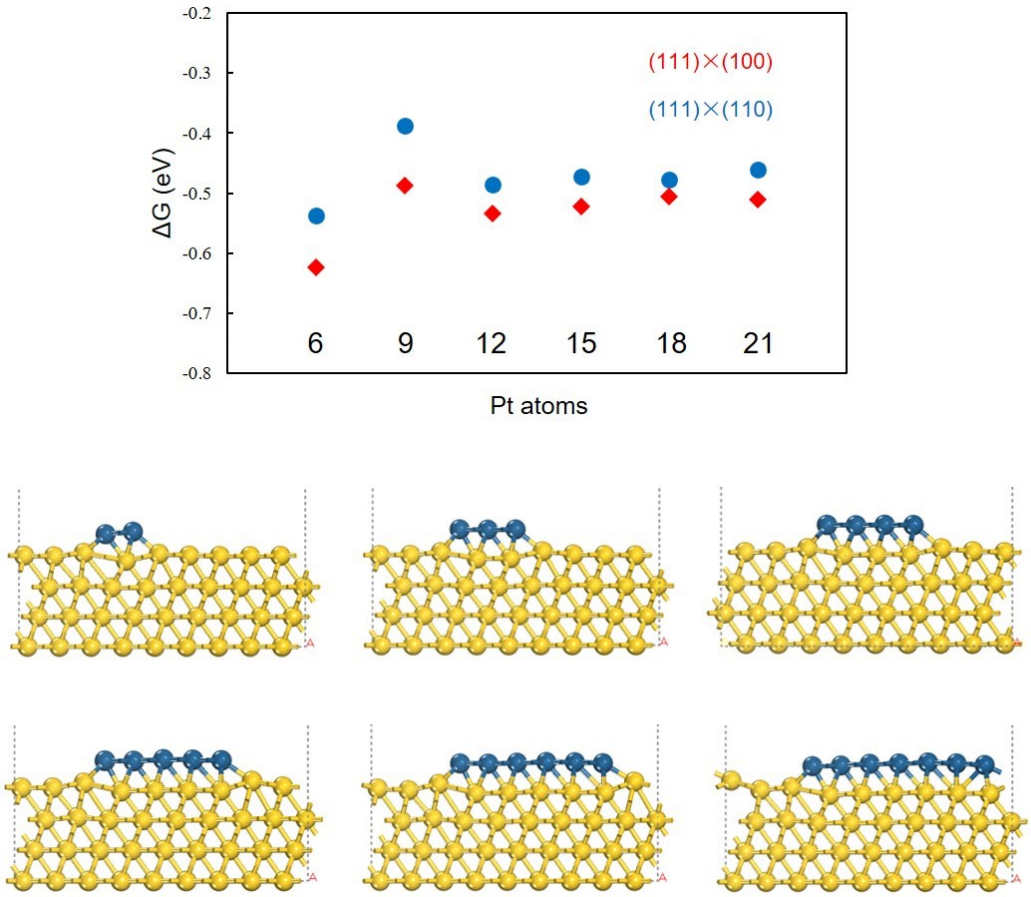


Fig. S1 Calculated H* adsorption energies (units in eV) at the stepped interface with different Pt coverage on Au(111).

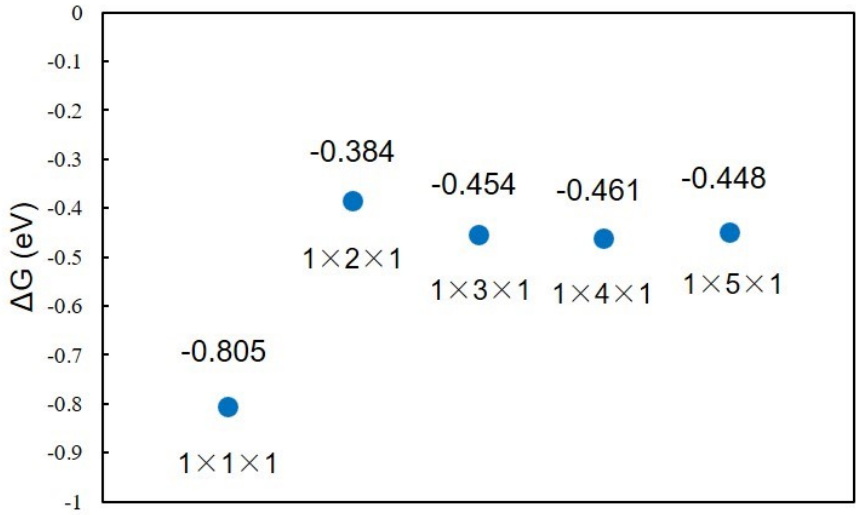


Fig. S2 Calculated Gibbs free energy of the reaction, $CH_3CH_2OH \rightarrow CH_3CHOH^* + H^*$, with different Monkhorst-Pack *k*-point sampling at the (111)×(110) interface.

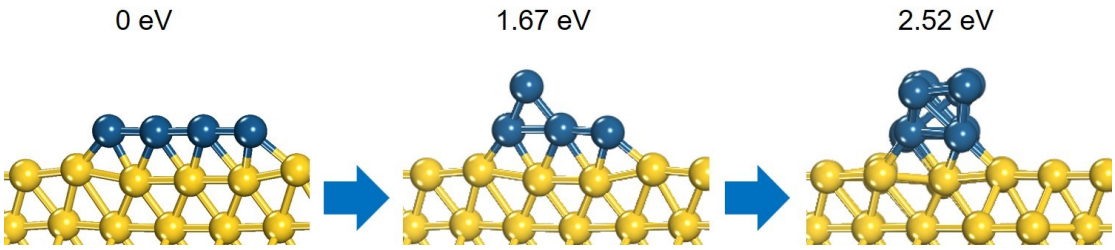
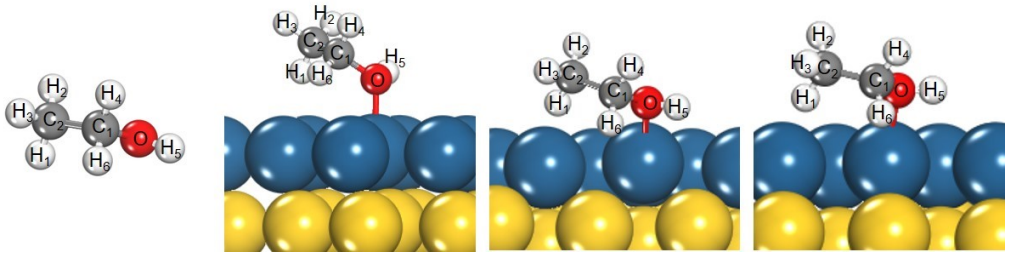


Fig. S3 The stability of the Pt/Au(111) interface model in thermodynamics.



atom	vacuum	(111) terrace	(111)×(110) interface	(111)×(100) interface
C_1	+0.38	+0.27	+0.33	+0.32
C_2	-0.12	-0.11	-0.12	-0.08
H_1	+0.04	+0.08	+0.05	+0.02
H_2	+0.06	+0.03	+0.06	+0.09
H_3	+0.05	+0.07	+0.07	+0.04
H_4	+0.05	+0.09	+0.09	+0.10
H_5	+0.63	+0.64	+0.61	+0.66
H_6	+0.06	+0.11	+0.08	+0.07
O	-1.15	-1.07	-1.04	-1.10
total	0	+0.12	+0.12	+0.12

Fig. S4 Bader charge analysis of each atom (units in e) in the ethanol molecule in vacuum and over the flat (111) terrace and stepped (111)×(110) and (111)×(100) interfaces on Pt/Au(111).

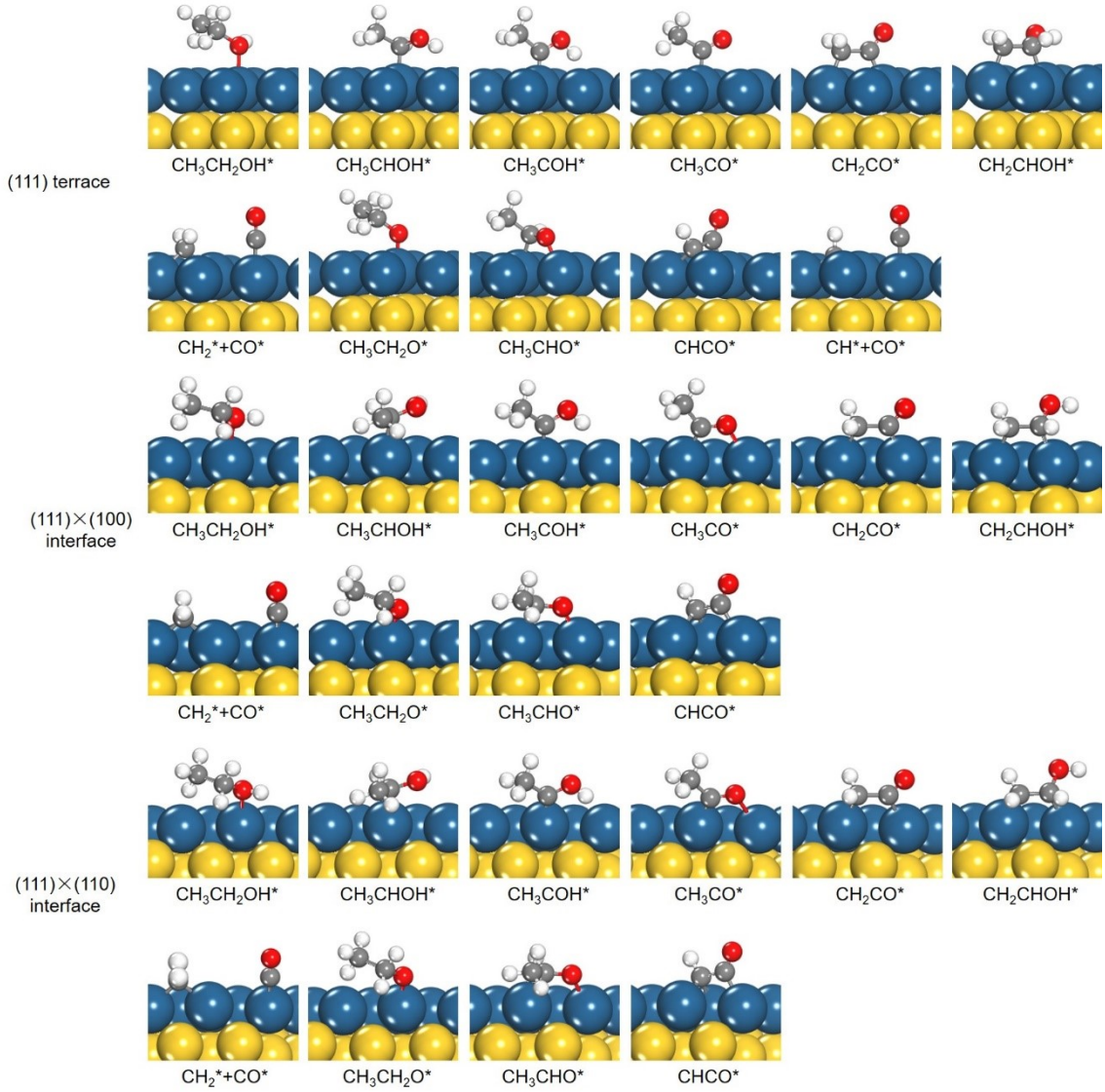


Fig. S5 Side views of optimized structures of intermediates over the flat (111) terrace and stepped (111)×(100) and (111)×(110) interfaces on Pt/Au(111).

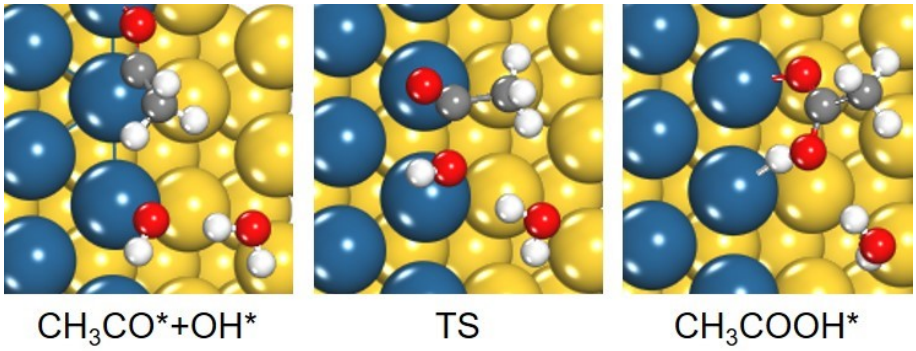


Fig. S6 Optimized structures of CH_3CO^* + OH*, the transition states and CH_3COOH^* on the (111)×(100) interface with one water molecule near the OH*.

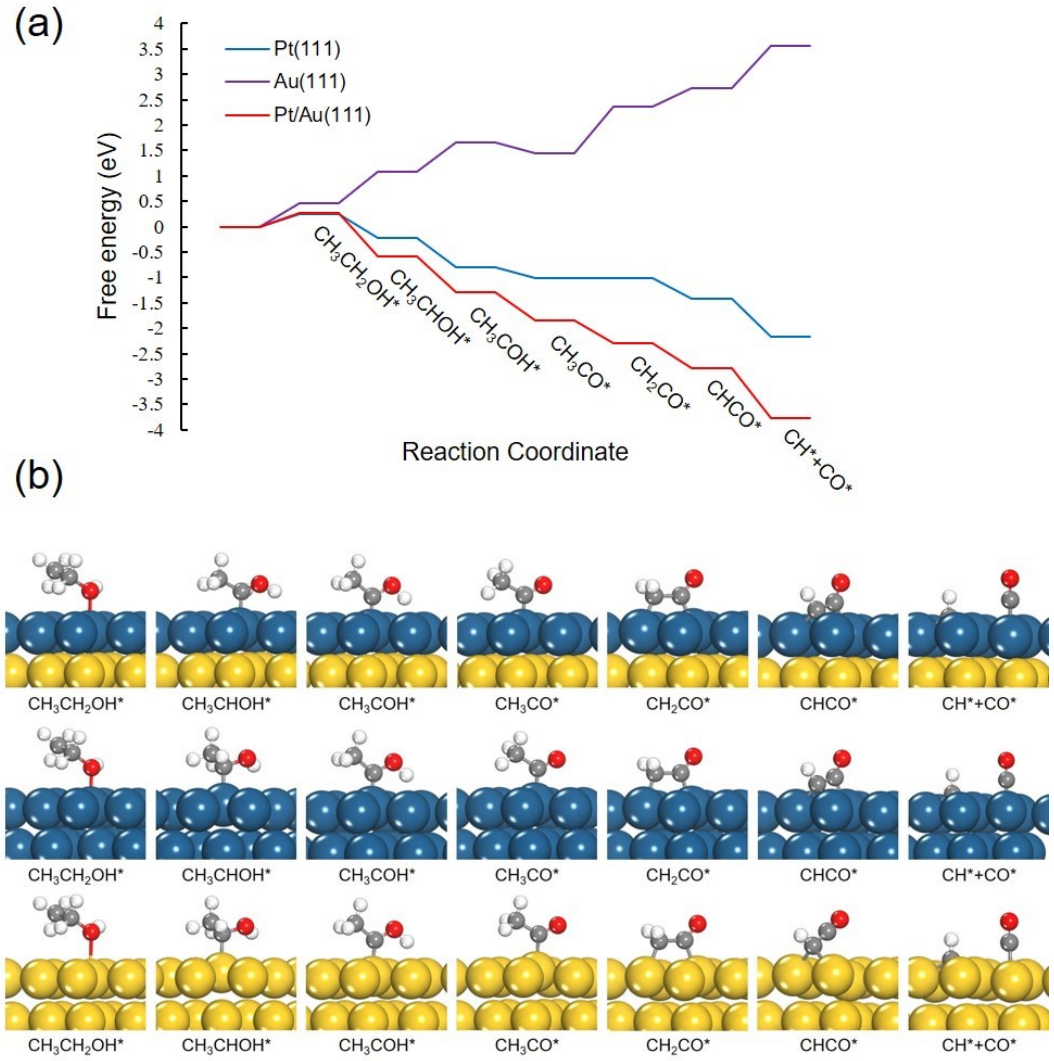


Fig. S7 (a) Comparison of Gibbs free energy profiles for ethanol decomposition on Pt(111), Au(111) and Pt/Au(111). (b) Optimized structures of intermediates on Pt(111), Au(111) and Pt/Au(111).