Supporting information

A DFT Study of Furfural Conversion on Re/Pt Bimetallic Surface: Synergetic Effect on the Promotion of Hydrodeoxygenation

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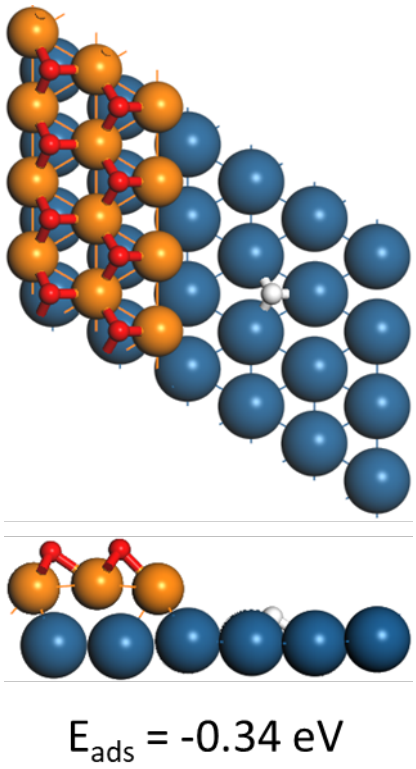

Figure S1: Adsorption of hydrogen atom on Re/Pt bimetallic system.

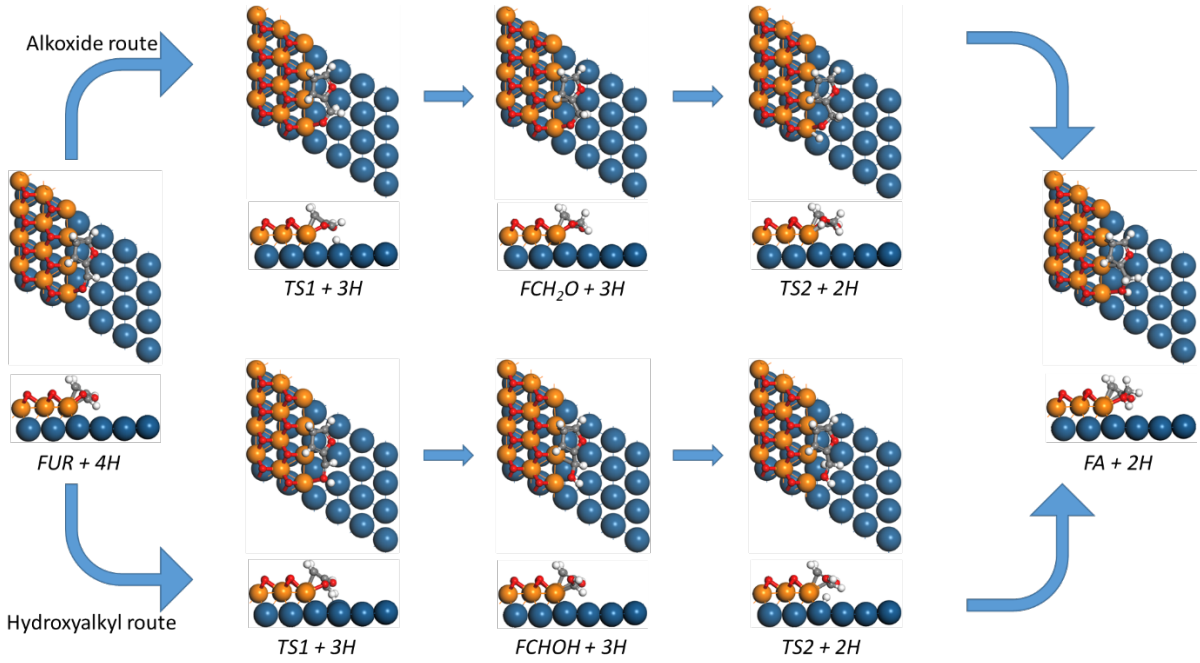

Figure S2: Mechanisms of furfural conversion to furfuryl alcohol.

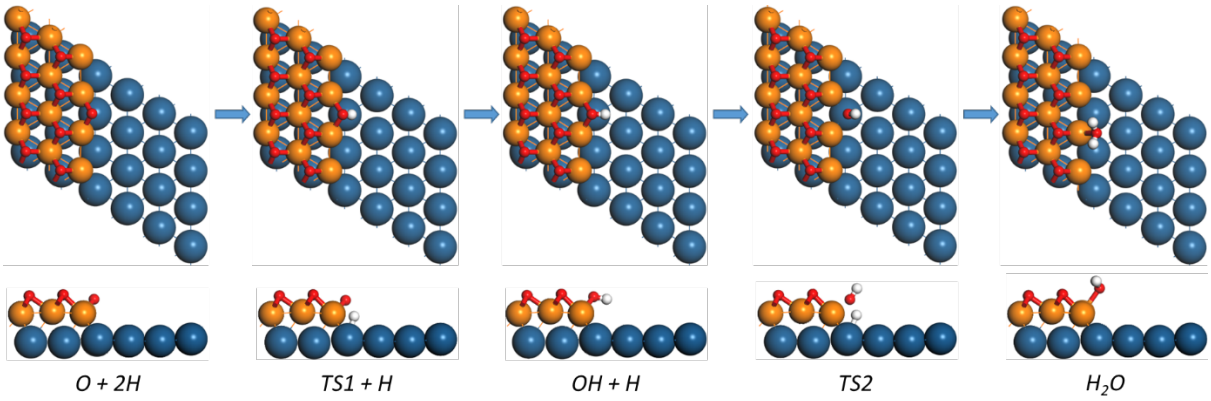

Figure S3: Mechanism of successive hydrogenations of oxygen into water.

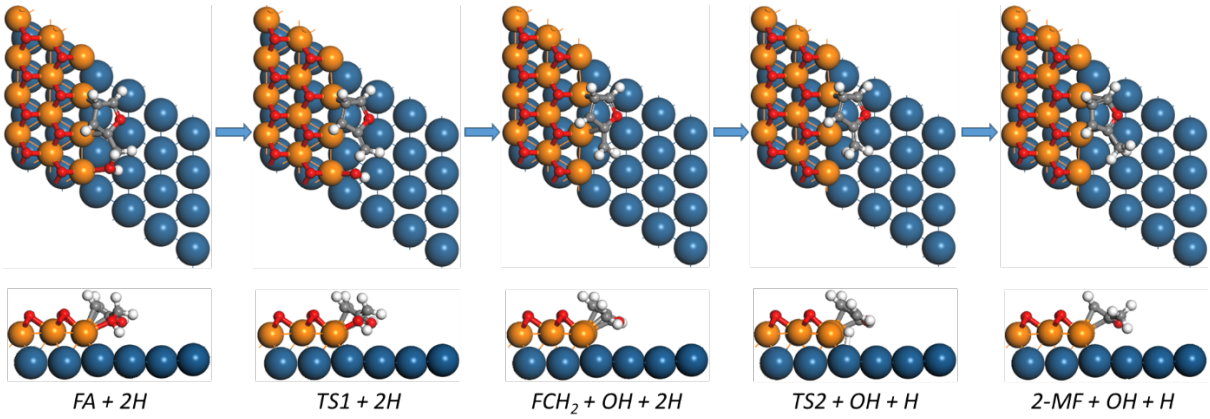

Figure S4: Mechanism of 2-methylfuran formation via direct cleavage of C-OH bond of furfuryl alcohol.

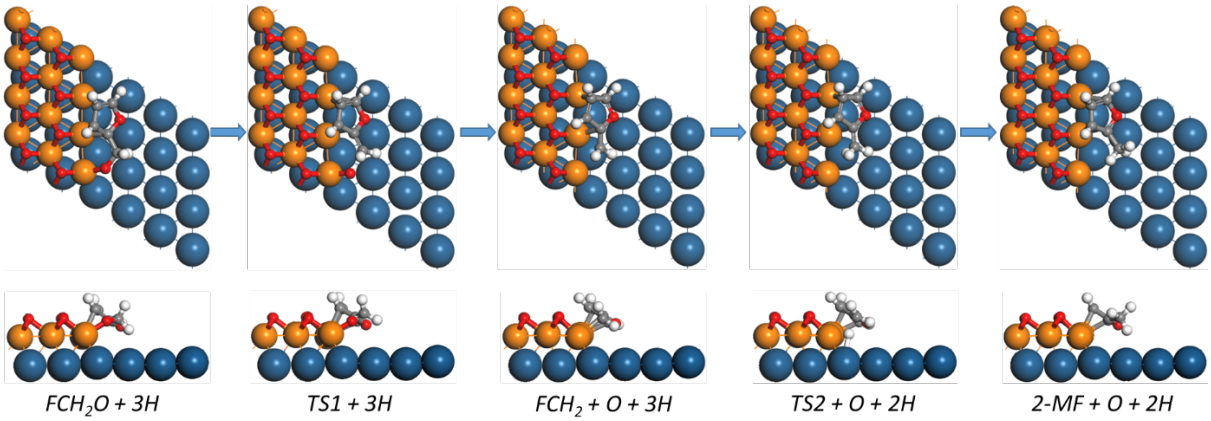

Figure S5: Mechanism of 2-methylfuran formation via the cleavage of C-O bond of alkoxide intermediate.

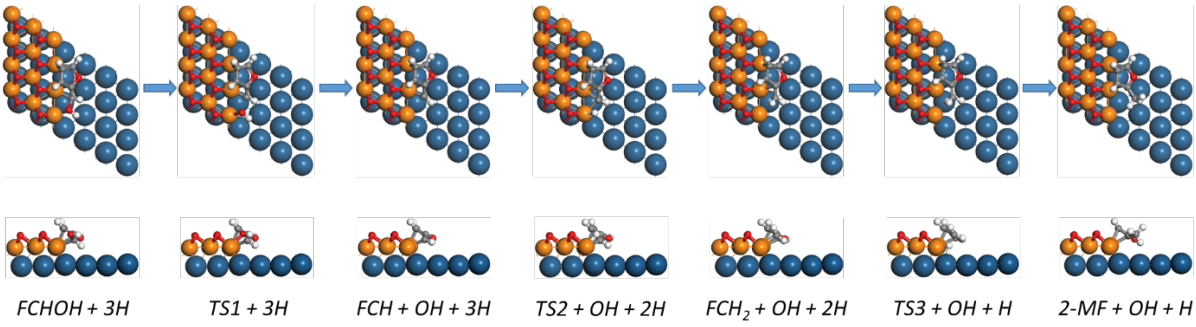

Figure S6: Mechanism of 2-methylfuran formation via the cleavage of C-OH bond of hydroxyalkyl intermediate.

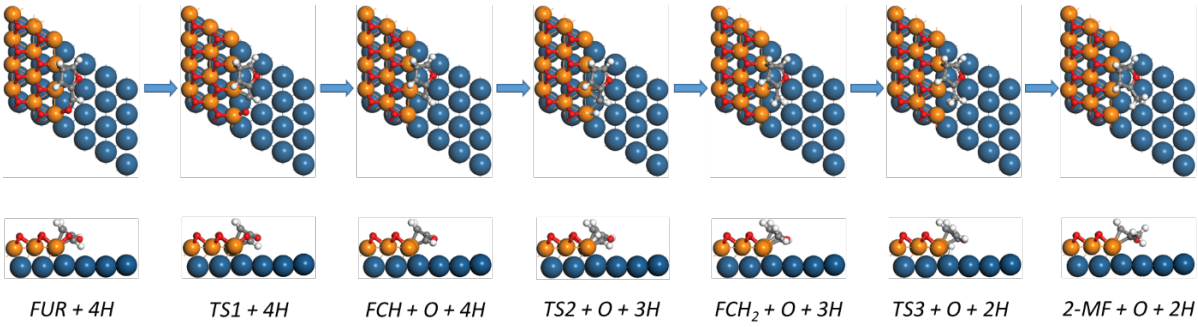

Figure S7: Mechanism of 2-methylfuran formation via the direct cleavage of C-O bond of furfural.

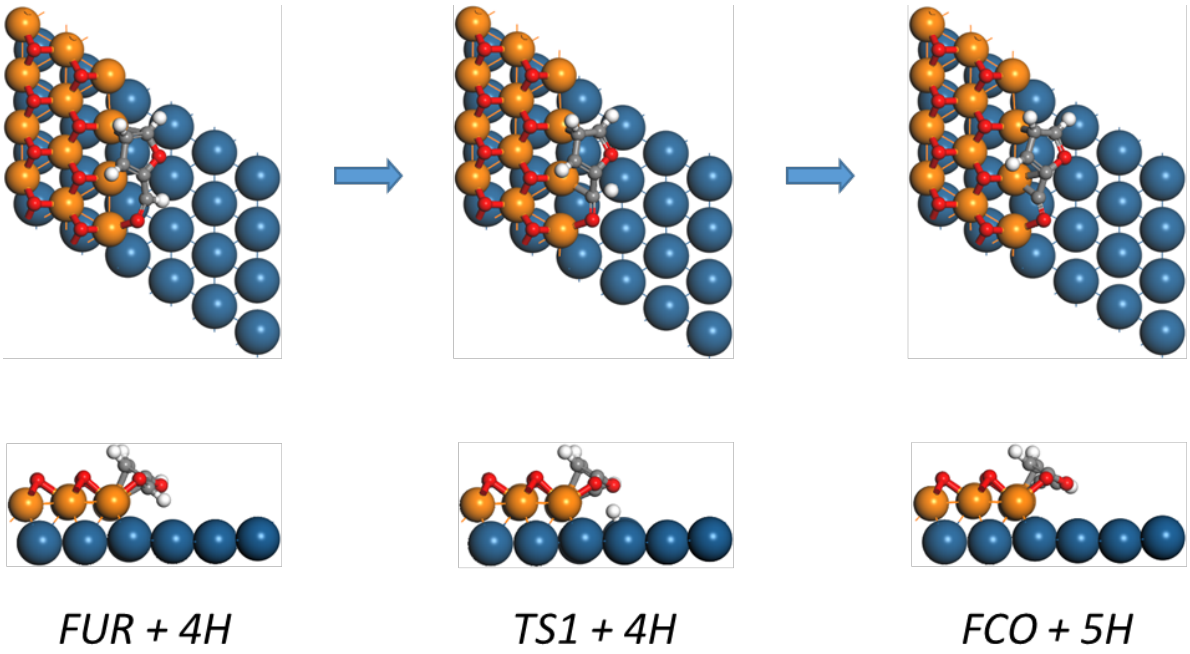

Figure S8: Mechanism of furfural dehydrogenation.

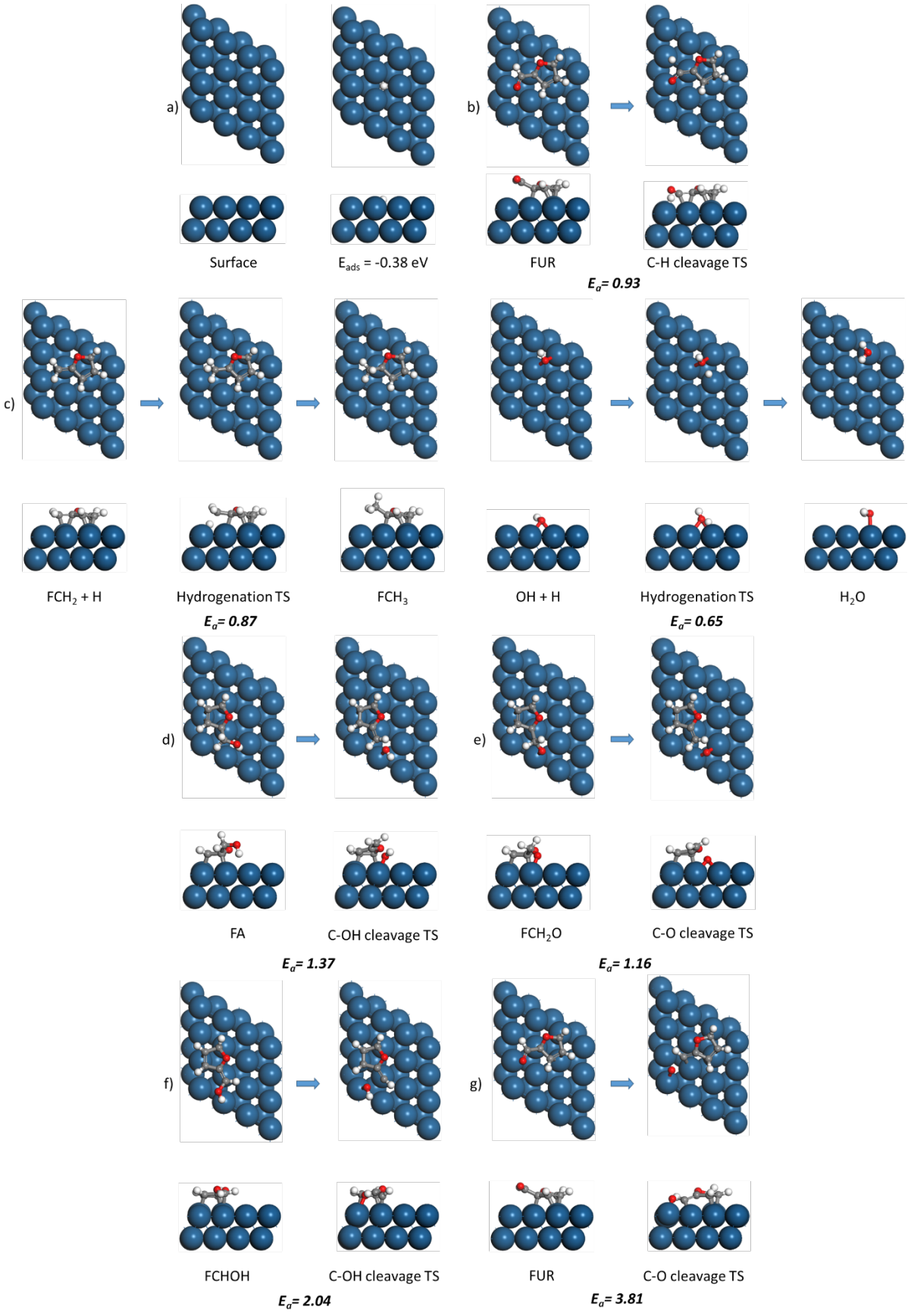
a)
b)
Surface
E_{ads} = -0.38 eV
FUR
C-H cleavage TS
E_a= 0.93
c)
FCH_2 + H
Hydrogenation TS
E_a= 0.87
FCH_3
OH + H
Hydrogenation TS
E_a= 0.65
H_2O
d)
e)
FA
C-OH cleavage TS
E_a= 1.37
FCH_2O
C-O cleavage TS
E_a= 1.16
f)
g)
FCHOH
C-OH cleavage TS
E_a= 2.04
FUR
C-O cleavage TS
E_a= 3.81

Figure S9: Key steps of furfural hydrodeoxygenation reaction structures on Pt(111). a) shows the Pt(111) surface with single hydrogen atom adsorption energy. b) shows the initial C-H cleavage barrier of furfural. c) shows the hydrogenation barriers of FCH_2 to 2-methylfuran and hydroxyl to water. d), e), f) and g) shows the C-O cleavage barrier of furfuryl alcohol, FCH_2O, FCHOH, and furfural respectively.