Supporting Information

Ru–Support Interface Tailoring for Enhanced Aerobic Oxidation of 1,4-Butanediol

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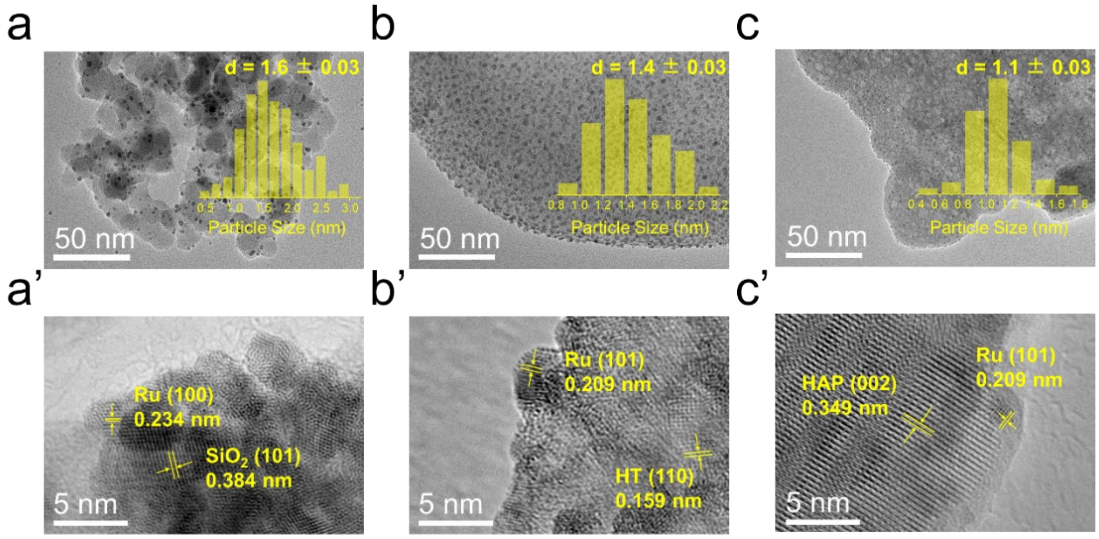

Figure S1. TEM and HRTEM images of Ru/SiO_2 (a-a'), Ru/HT (b-b'), Ru/HAP (c-c').

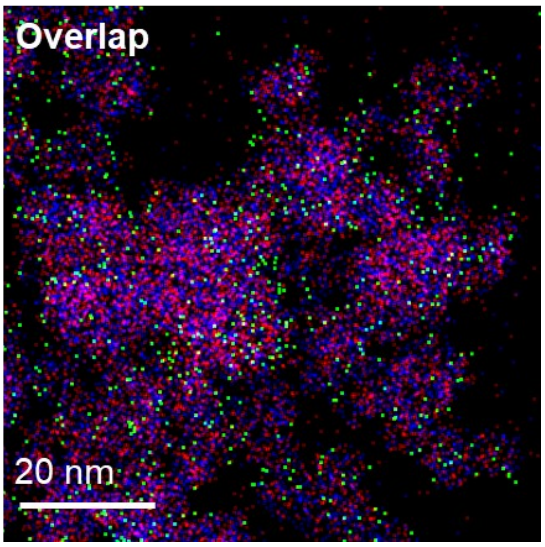

Figure S2. Overlay of Ru, Ti, and O elemental maps obtained by STEM-EDX analysis.

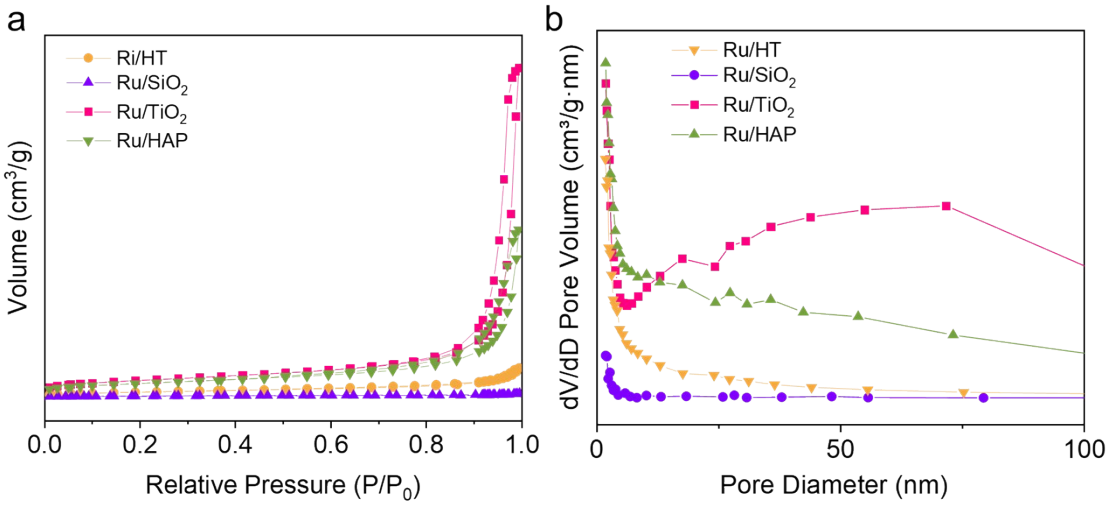

Figure S3. (a) N_2 adsorption–desorption isotherms of the Ru–Support Interface catalyst. (b) Pore size distribution plot.

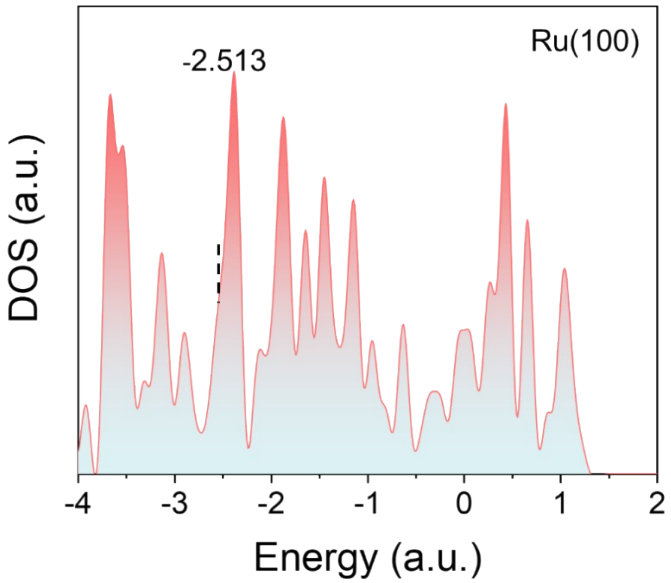

Figure S4. Analysis of DOS of Ru(100) model surface.

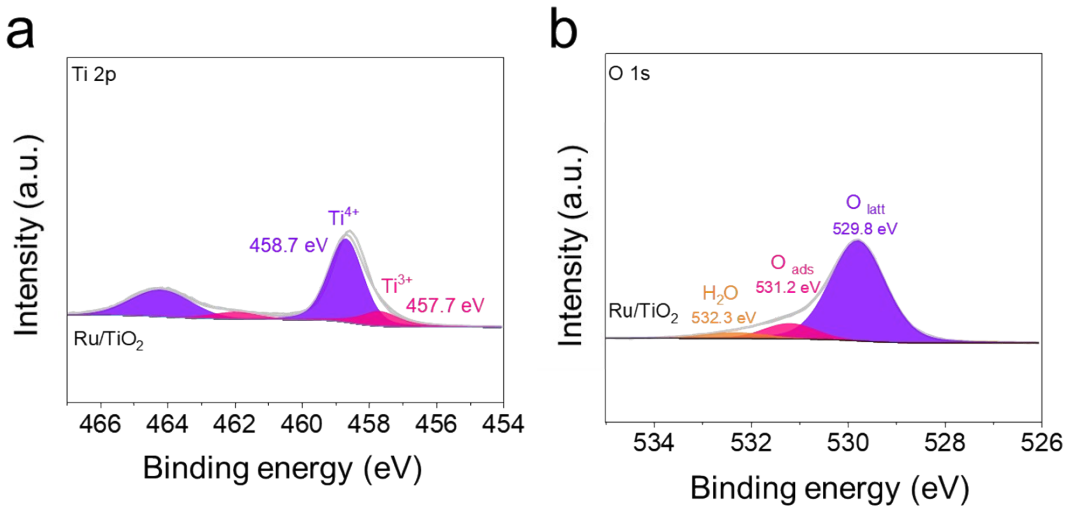

Figure S5. (a) Ti 2p and (b) O 1s XPS spectra of the Ru/TiO_2 catalyst.

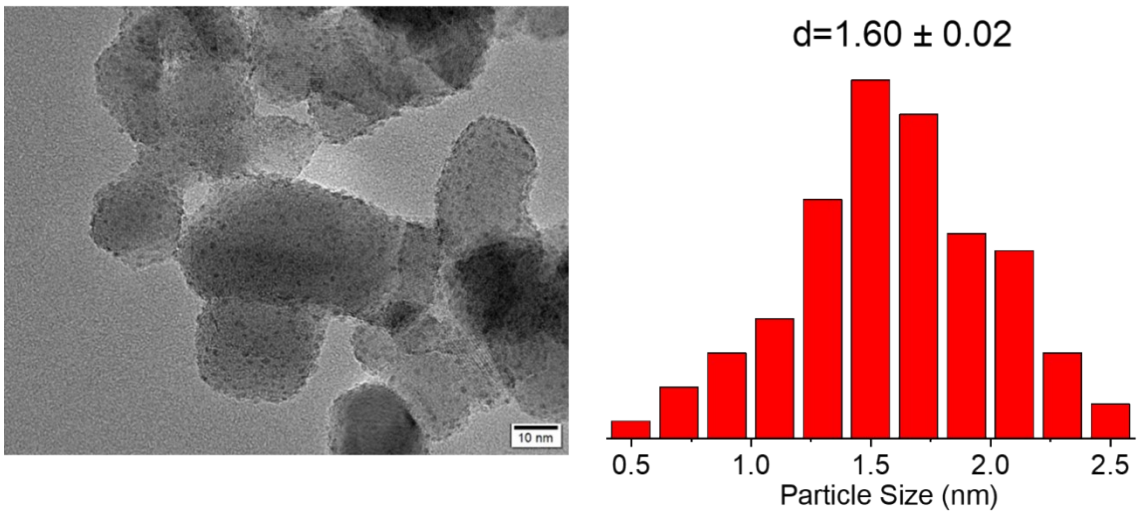

Figure S6. TEM image of Ru/TiO_2 after reaction and the corresponding partial size.

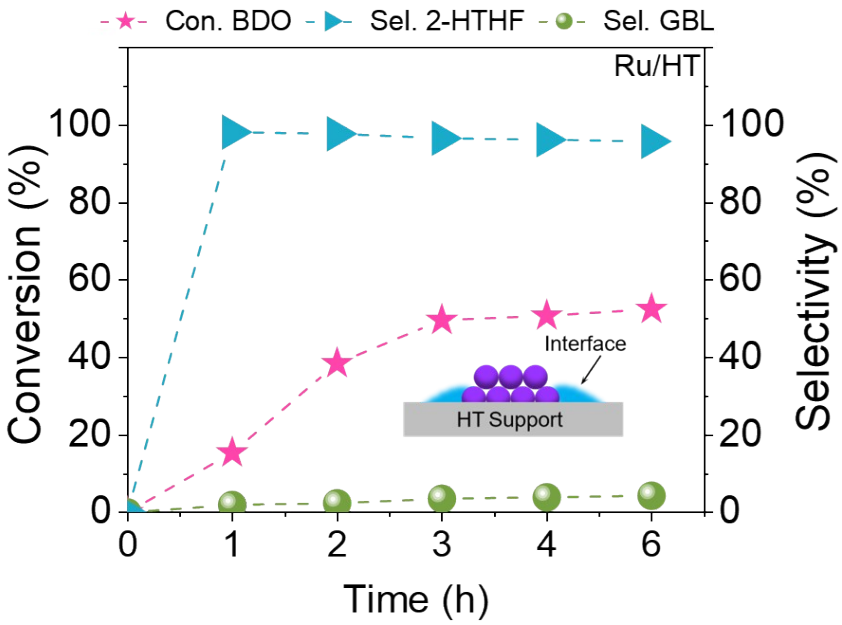

Figure S7. Kinetic Study of the Ru/HT catalyst.

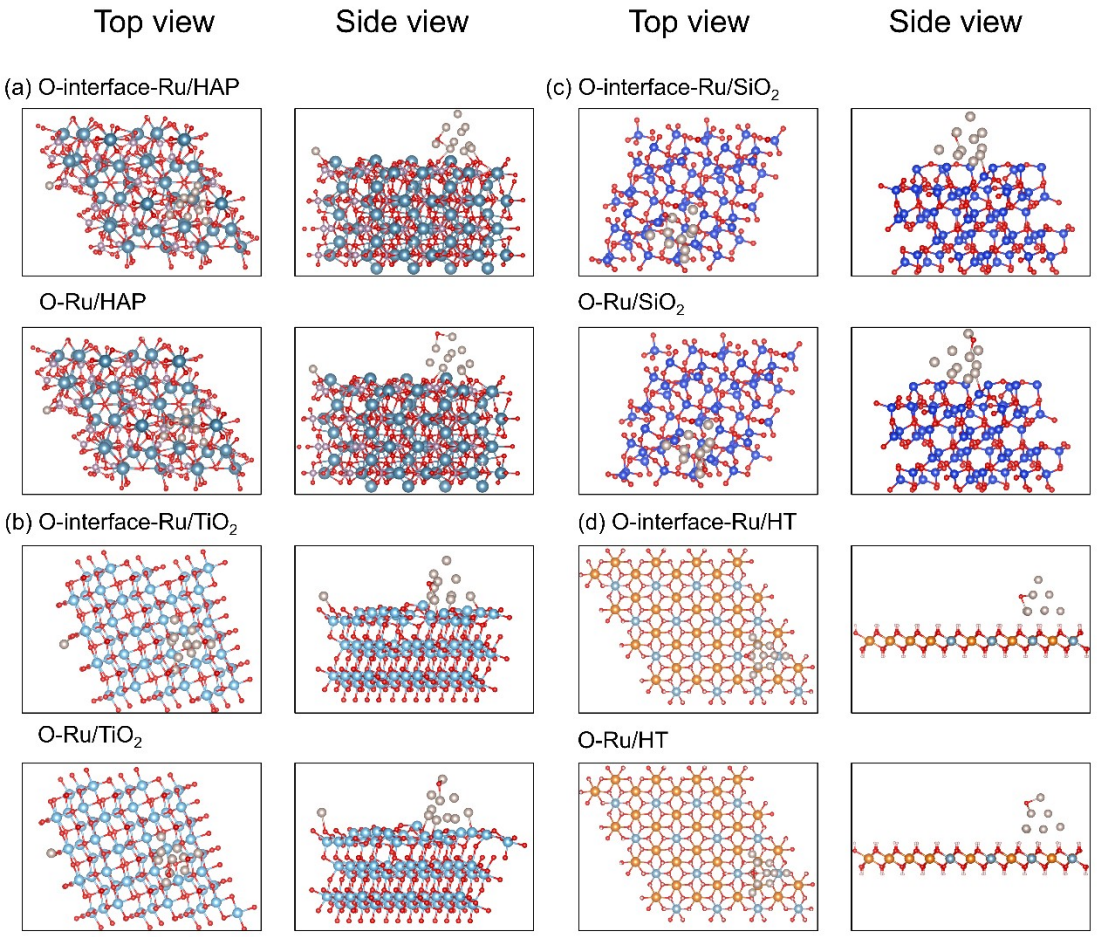

Figure S8. Top and side views of adsorption geometries of O atom on (a) Ru/HAP, (b) Ru/TiO_2, (c) Ru/SiO_2, (d) Ru/HT model surface, respectively.

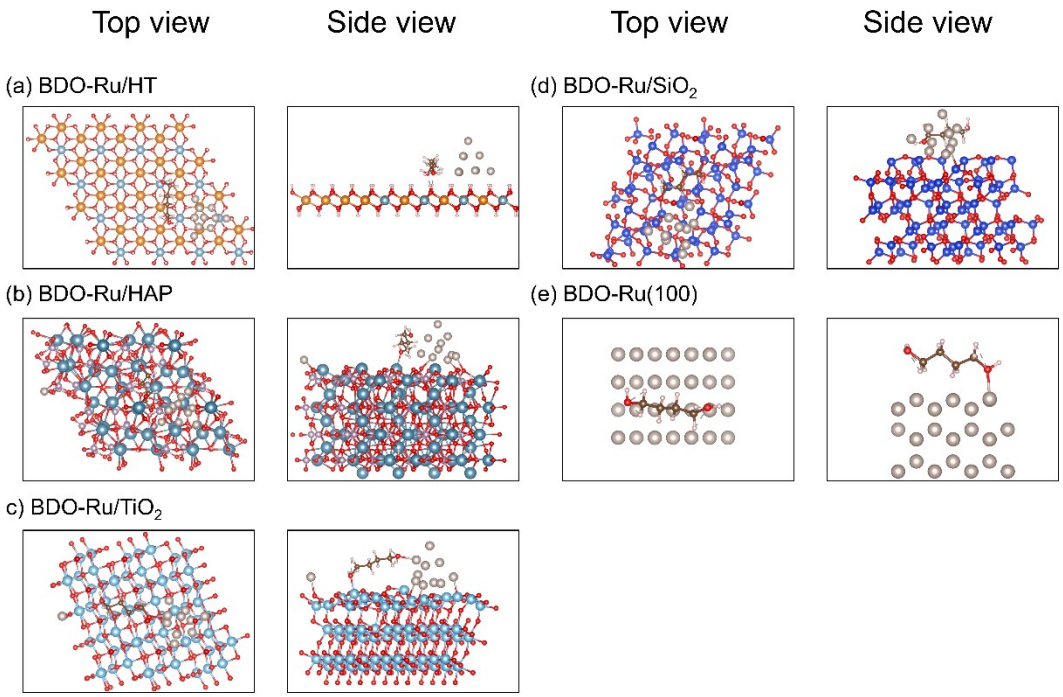

Figure S9. Top and side views of adsorption geometries of BDO on (a) Ru/HAP, (b) Ru/TiO_2, (c) Ru/SiO_2, (d) Ru/HT, (e) Ru(100) model surface, respectively.

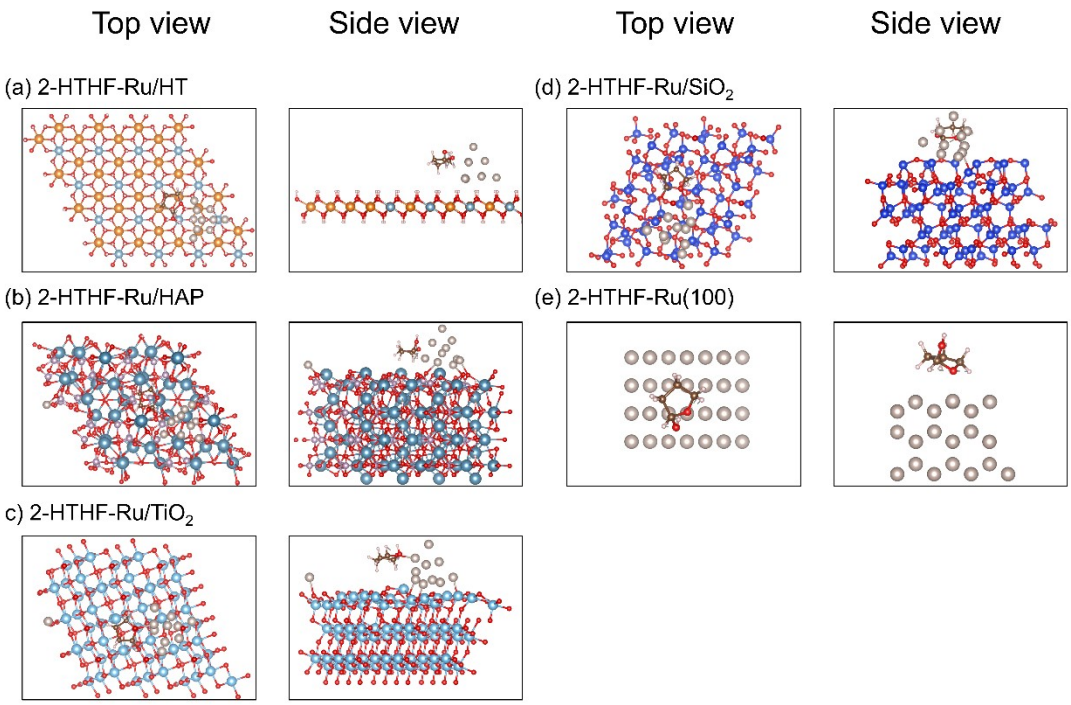

Figure S10. Top and side views of adsorption geometries of 2-HTHF on (a) Ru/HT, (b) Ru/HAP, (c) Ru/TiO_2, (d) Ru/SiO_2, (e) Ru(100) model surface, respectively.

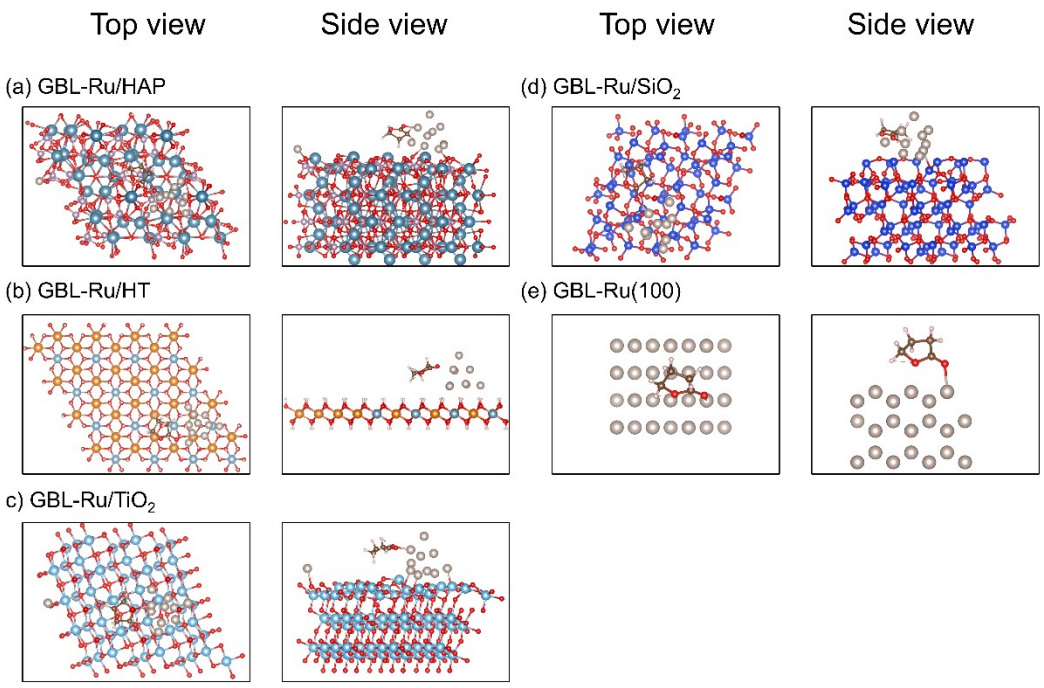

Figure S11. Top and side views of adsorption geometries of 2-HTHF on (a) Ru/HAP, (b) Ru/HT, (c) Ru/TiO_2, (d) Ru/SiO_2, (e) Ru(100) model surface, respectively.

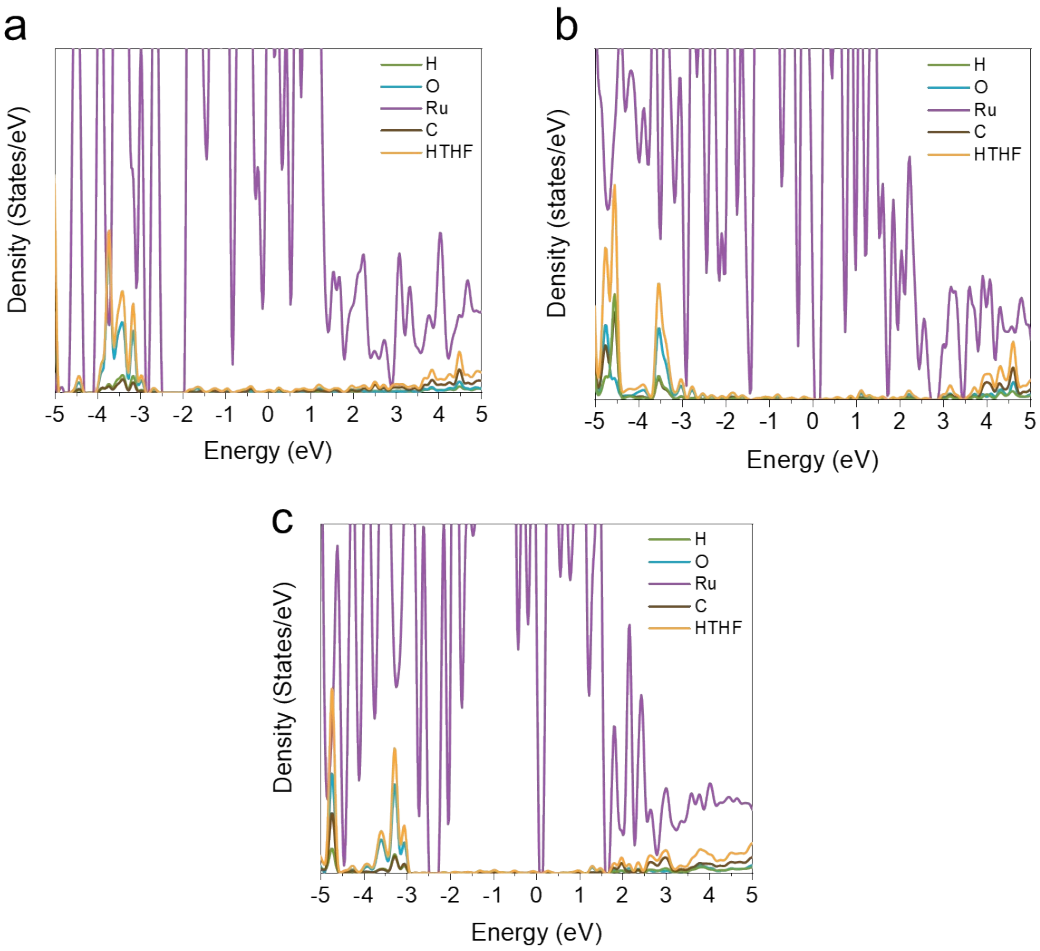

Figure S12. Density of states (DOS) of plots for (a) Ru/HT, (b) Ru/SiO_2, (c) Ru/HAP model surface, respectively.

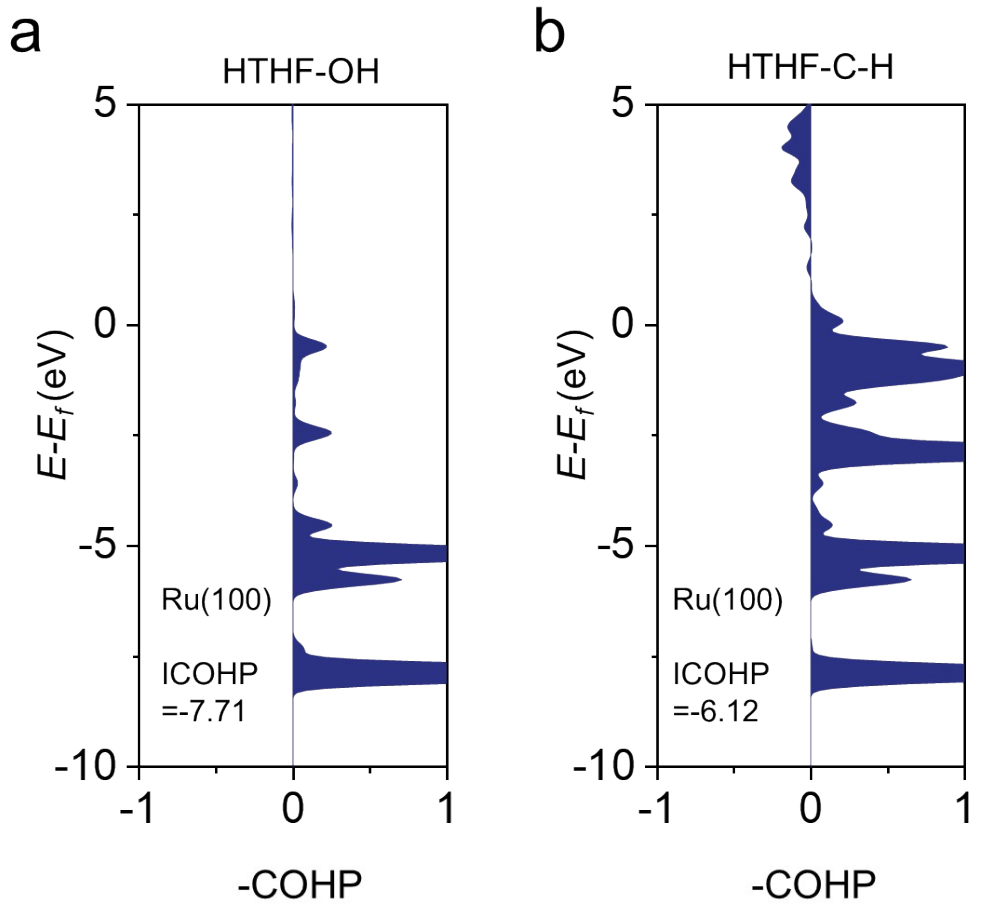

Figure S13. ICOHP values for the (a) O–H and (b) C–H bond in the adsorption configuration of 2-HTHF on the Ru(100) model surface, respectively.

Table S1 Structural properties and crystallite size of the different catalysts

Samples	Ru loading (wt %)[a]	Dispersion (%)[b]	Surface area ($m^2\ g^{-1}$)[c]	Pore diameter (nm)[c]	Pore volume (cm^2g^{-1})[c]
Ru/HT	3.93	19	3.93	9.90	0.000204
Ru/SiO_2	4.02	20	4.90	4.20	0.000389
Ru/TiO_2	4.17	16	61.5	34.3	0.002869
Ru/HAP	4.39	17	18.6	21.7	0.001354

[a]detected by inductively-coupled plasma optical emission spectroscopy (ICP-OES).

[b]Ru dispersion determined by CO pulse chemisorption.

[c]Surface area, pore diameter, and volume were determined by N_2 physisorption measurements.

Table S2 Comparison of catalyst performance of Ru/TiO_2 with the representative ones reported in the literature in terms of activity in the aerobic oxidation reaction of aliphatic alcohols.

Catalysts	Reaction condition	BDO Con. (%)	2-HTHF Sel. (%)	TOF (h^{-1})	References
Ru/HT	0.5 MPa,120 °C	52	96	451	This work
Ru/SiO_2	0.5 MPa,120 °C	66	93	552	This work
Ru/TiO_2	0.5 MPa,120 °C	99	97	1043	This work
Ru/HAP	0.5 MPa,120 °C	99	70	846	This work
Au/TiO_2	1.25 MPa,120 °C	>99	1	64	Ref.[1]
Au/α-Fe_3O_4	1.25 MPa, 140 °C	100	14	207	Ref.[2]
Pd/TiO_2	0.1 MPa, 90 °C	30	90	9	Ref.[3]
5%Pd/C	0.3 MPa, 50 °C	95	23	500	Ref.[4]
Pt/TiO_2	0.1MPa, 90 °C	30	15	405	Ref.[3]
Cu/Al_2O_3	0.1 MPa, 200 °C	100	2	18	Ref.[5]
Cu/MgO-CeO_2	0.1 Mpa, 240 °C	100	1	12	Ref.[6]
0.5%Cu-1.0%Pt/AC	0.1 MPa, 90 °C	80	31	437	Ref.[7]
Ru^{3+}-hydroxyapatite	0.1 MPa, 80 °C	95	6	0.4	Ref.[8]
PNP-type Ru (II)	0.1 MPa, 110 °C	96	4	17	Ref.[9]
1.4%Ru/Al_2O_3	0.1 MPa, 150 °C	none	none	300	Ref.[10]
$Ru_{0.35}MnFe_{1.5}Cu_{0.15}O_x$	0.1 MPa, 22 °C	90	0	3	Ref.[11]

Table S3 Catalytic performance of the catalysts with different Ru loadings

Ru loading (wt %)	BDO Con.%[a]	2-HTHF Sel.%	GBL Sel.%
2.0 wt%	65.3	95.1	4.9
4.0 wt%	76.9	94.6	5.4
6.0 wt%	99.0	96.7	3.3
8.0 wt%	94.3	98.3	1.7

[a] Reaction conditions: 100 mg BDO, 30 mg catalyst, 10 mL TBP, 120 ^{o}C, 0.5 MPa O_2, 6h, 800 rpm.

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