Electronic supplementary information for

Double-active site synergistic catalysis in Ru-TiO_2 toward benzene hydrogenation to cyclohexene with largely enhanced selectivity

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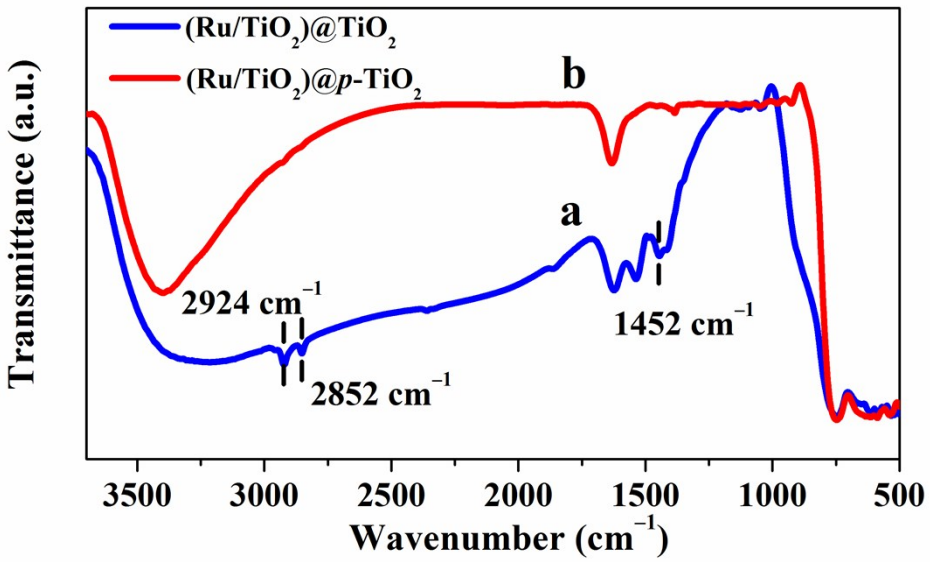

Fig. S1 FTIR spectra of (a) $(Ru/TiO_2)@TiO_2$ and (b) $(Ru/TiO_2)@p\text{-}TiO_2$.

Table S1. Catalytic performance of various catalysts

Catalysts	Additive	Conv. (%)	S_{CHE} (%)	Y_{CHE} (%)	Ref.
Ru/TiO_2	-	73.1	32.6	23.8	This work
$(Ru/TiO_2)@p\text{-}TiO_2$	-	98.1	76.6	75.1	This work
$Ru/ZnO\text{-}ZrO_x(OH)_y$	-	77.5	72.3	56.0	[1]
$Ru_{1.0}Cu_{0.5}/MgAl\text{-}LDH$	-	71.8	61.3	44.0	[2]
$RuCoB/\gamma\text{-}Al_2O_3$	-	62.7	45.7	28.8	[3]
$Ru\text{-}Zn/HfO_2$	$ZnSO_4$	60.0	82.8	49.7	[4]
$Ru–La–B/ZrO_2$	$ZnSO_4$	80.8	66.5	53.7	[5]
Ru/BEN (IP-HY)	$ZnSO_4$	61.5	45.2	27.8	[6]
Ru-Zn/HAP-1	$ZnSO_4$	69.8	47.3	33.0	[7]
$Ru/B\text{-}ZrO_2$	$ZnSO_4$	80.0	60.0	48.0	[8]
Ru/P25	$ZnSO_4$	88.0	69.0	61.0	[9]

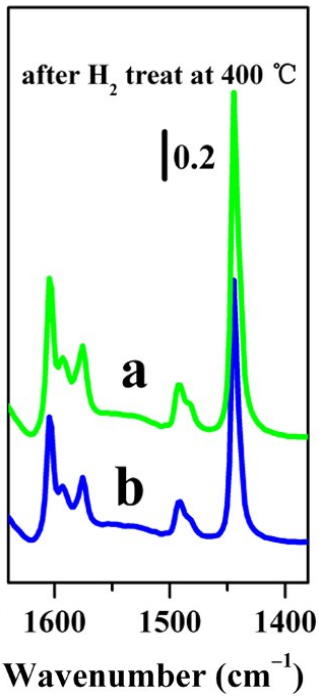

Fig. S2 Py-IR spectra of: (a) Ru/TiO_2 and (b) $(Ru/TiO_2)@p\text{-}TiO_2$ after H_2 treatment at 400 ºC.

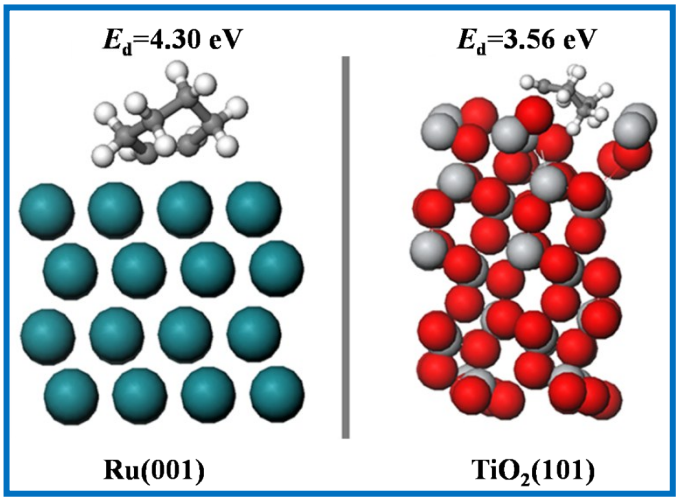

Fig. S3 Calculated adsorption models of cyclohexene on the typical Ru(001) and $TiO_2(101)$ facet, respectively.

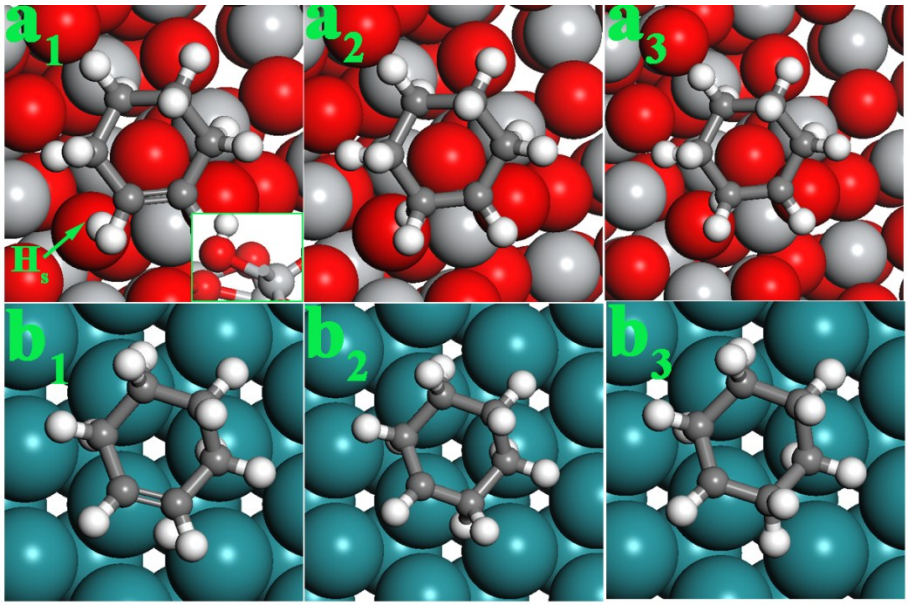

Fig. S4 Calculated hydrogenation models of cyclohexene with one hydrogen atom to C_6H_{11} over (a) TiO_2(101) facet and (b) Ru(001) facet, respectively. (a_1, b_1) Initial states, (a_2, b_2) transient states and (a_3, b_3) final states. Pale gray, red, blue balls are Ti, O and Ru, respectively.

References:

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