Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Geometric effect in the highly selective hydrogenation of 3-methylcrotonaldehyde over Pt@ZIF-8 core-shell catalyst

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Additional data: Figure S1-S10, Table S1-S2

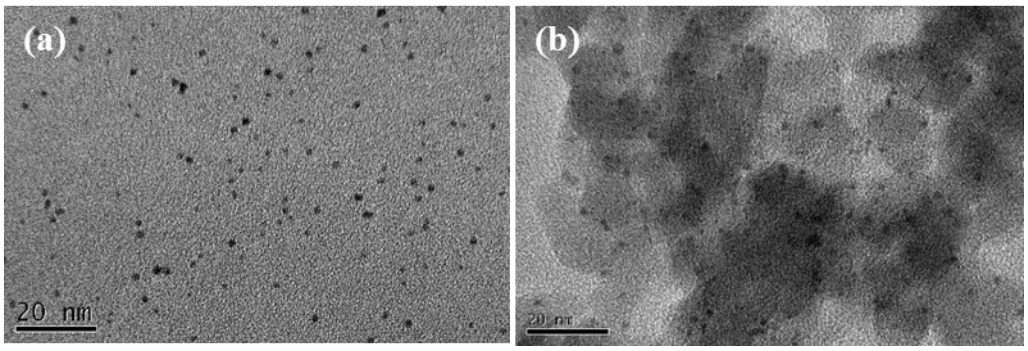


Fig. S1. TEM image of (a) Pt NPs and (b) Pt-0.23/SiO_2.

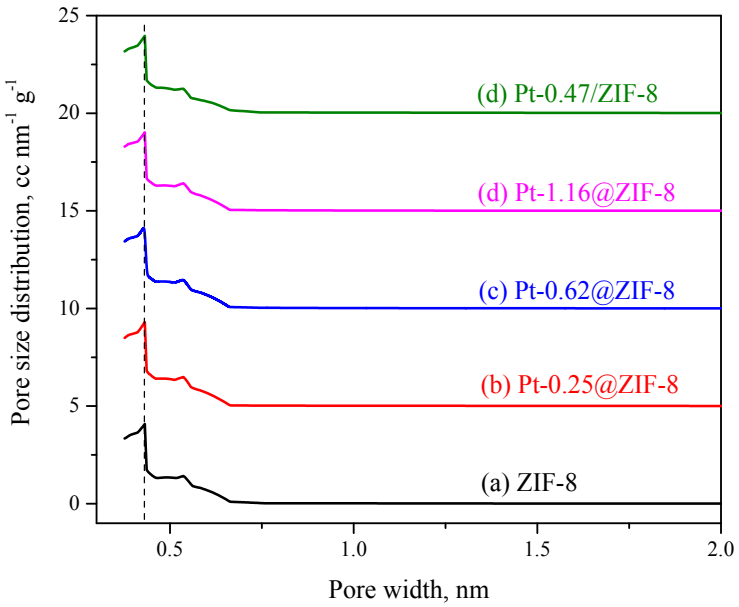
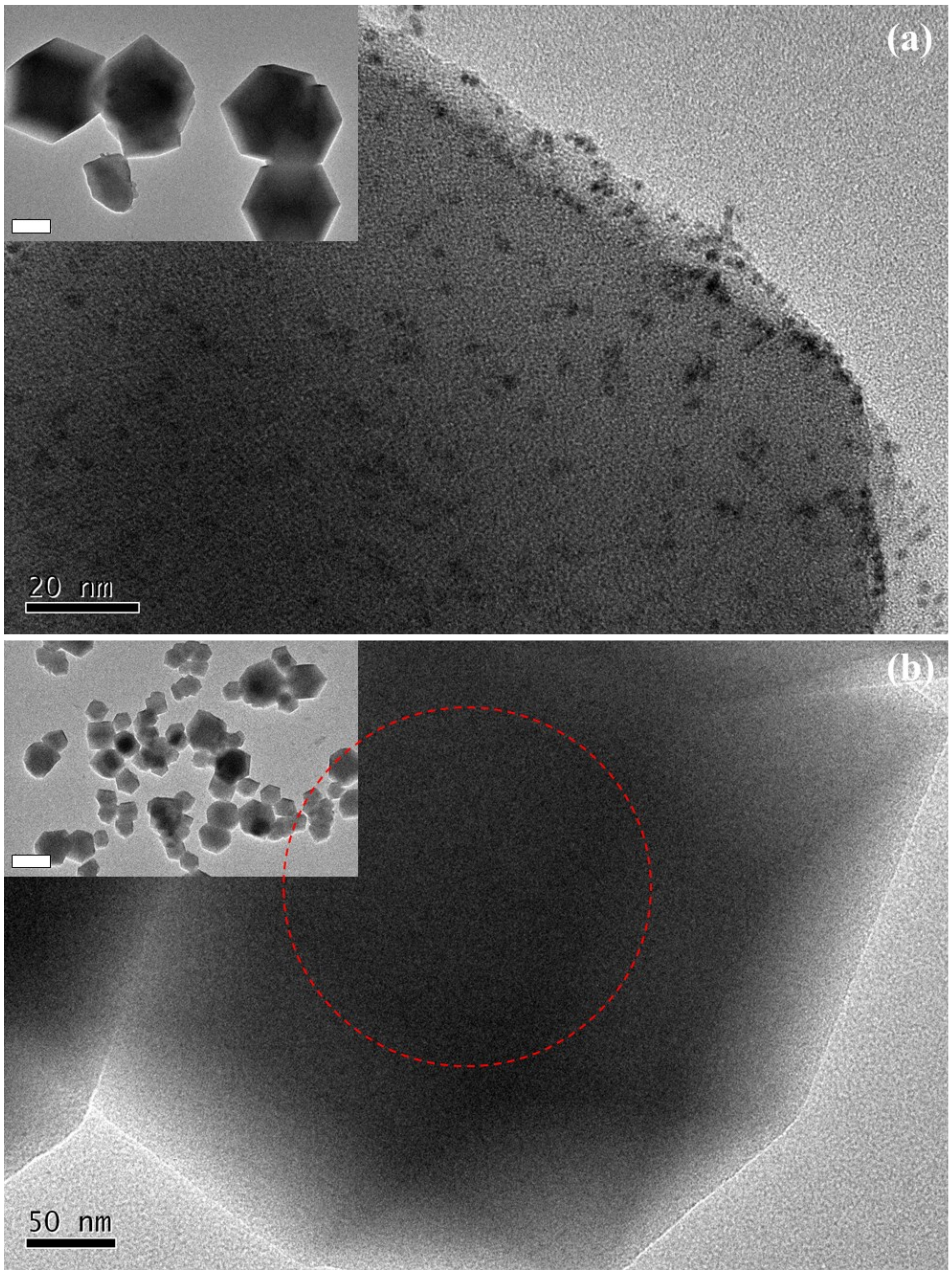


Fig. S2. Pore size distribution of the catalysts calculated by the HK method.


(a)
20 nm
(b)
50 nm

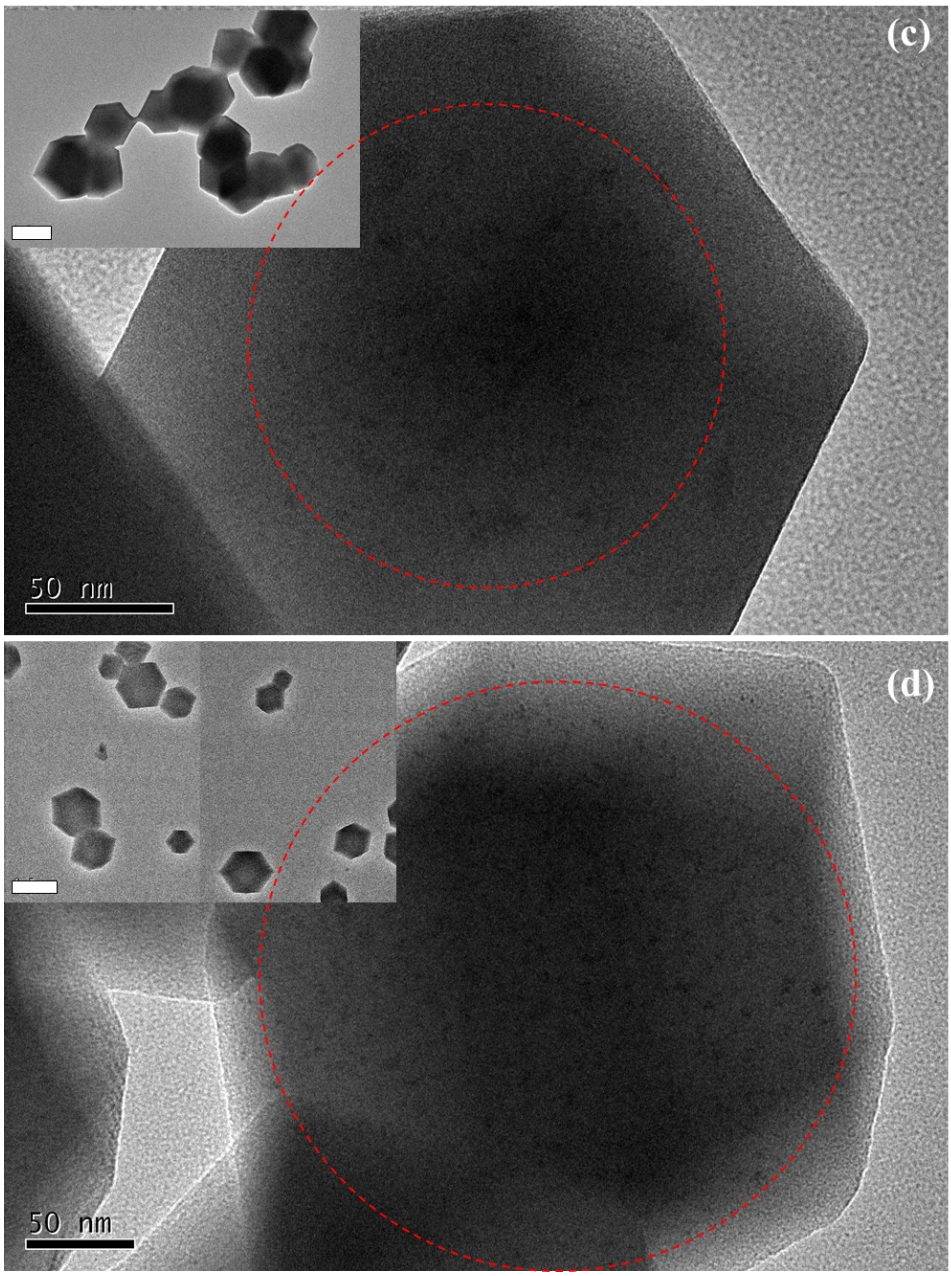


Fig. S3. TEM images of the catalysts: (a) Pt-0.47/ZIF-8, (b) Pt-0.25@ZIF-8, (c) Pt-0.62@ZIF-8, and (d) Pt-1.16@ZIF-8. (White scale bar: 0.5 μm)

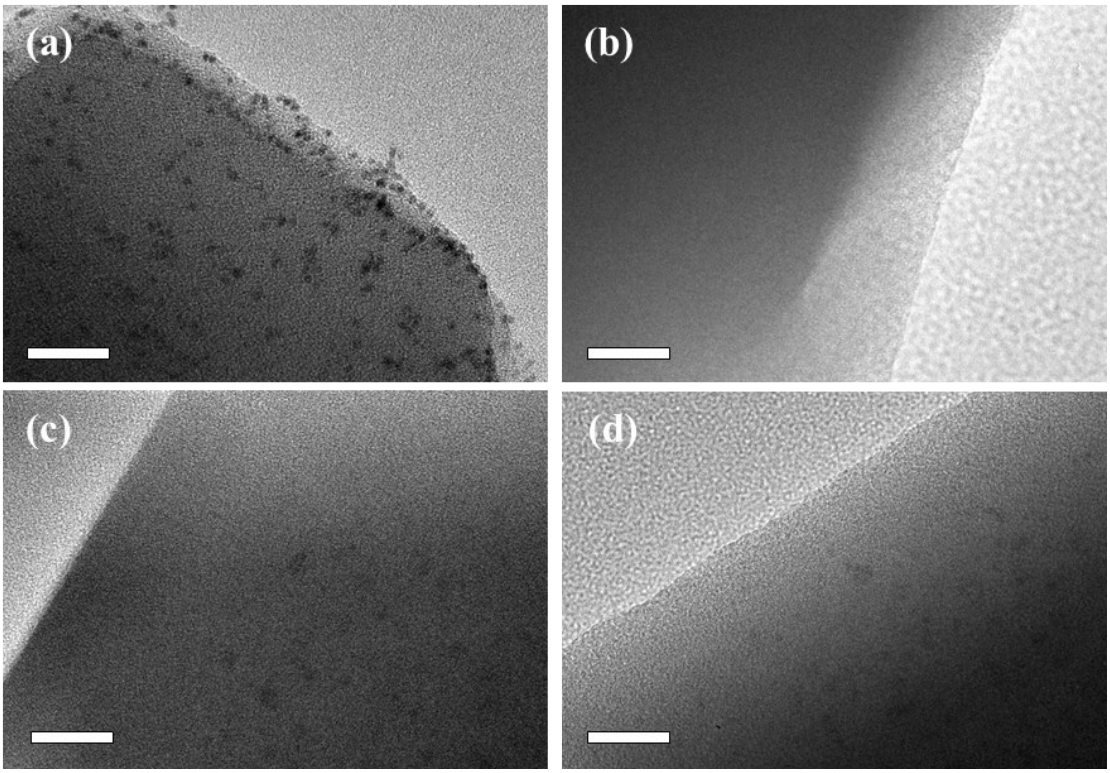


Fig. S4. HRTEM images of the fringes of the catalysts: (a) Pt-0.47/ZIF-8, (b) Pt-0.25@ZIF-8, (c) Pt-0.62@ZIF-8, and (d) Pt-1.16@ZIF-8. (Scale bar: 20 nm)

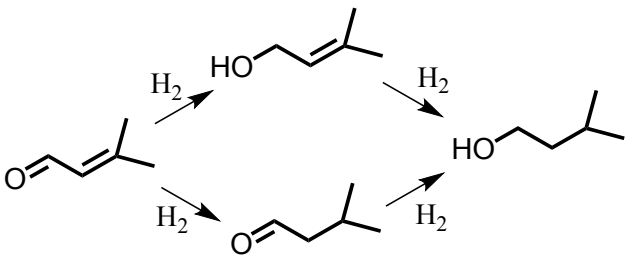
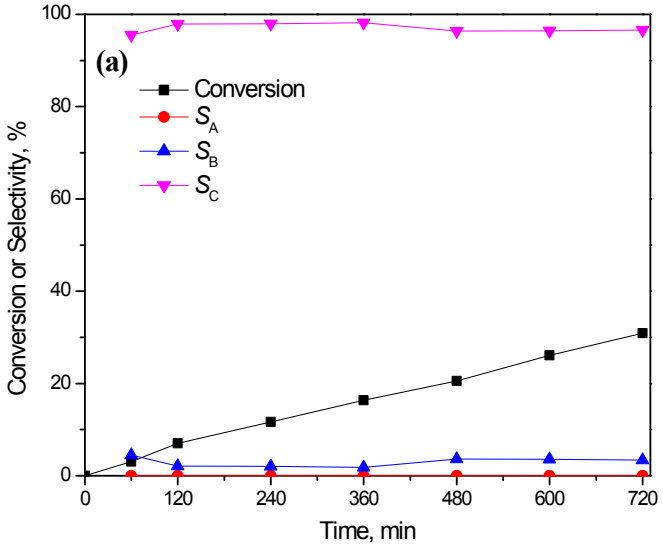


Fig. S5. Reaction pathway of the 3-methylcrotonaldehyde hydrogenation.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S_B
S_C
Conversion or Selectivity, %
Time, min
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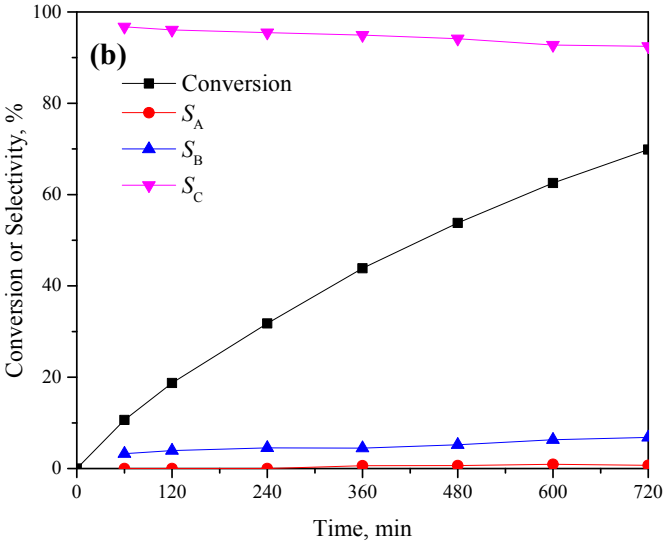
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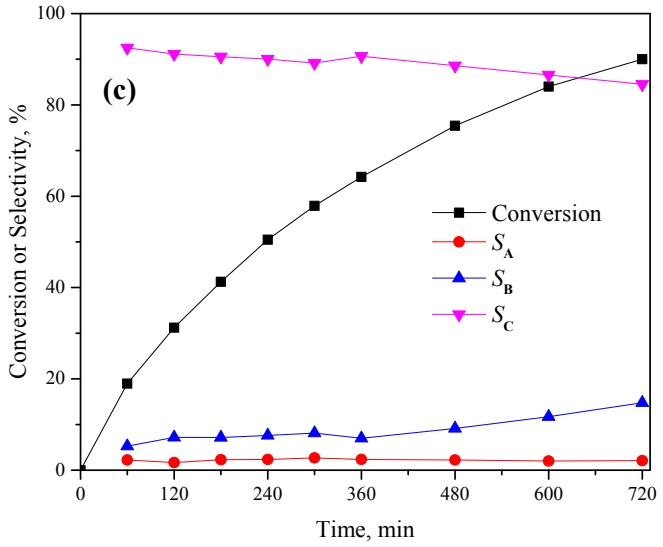
(c)
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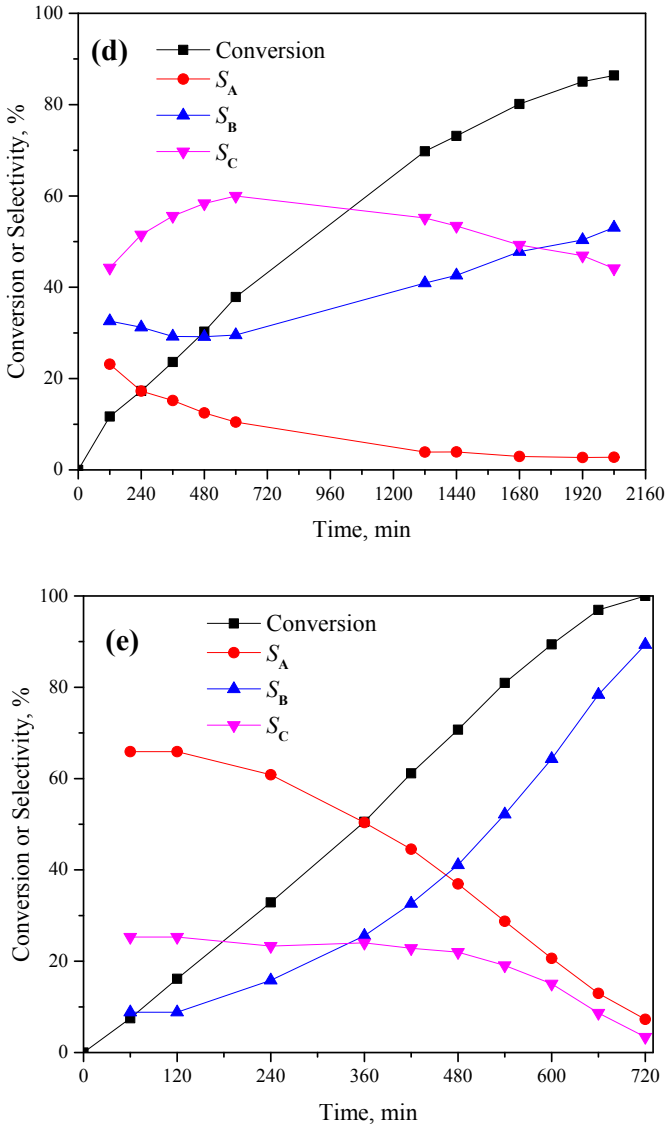


Fig. S6. Hydrogenation of 3-methylcrotonaldehyde over the catalysts (a) Pt-0.25@ZIF-8, (b) Pt-0.62@ZIF-8, (c) Pt-1.16@ZIF-8, (d) Pt-0.47/ZIF-8 and (e) Pt-0.23/SiO_2. The products are 3-methyl-1-butanal (**A**), 3-methyl-1-butanol (**B**) and prenol (**C**). The reaction conditions for Pt/SiO_2: 0.5 g catalyst, 0.5 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa; the reaction conditions for Pt@ZIF-8 and Pt/ZIF-8: 1.2 g catalyst, 0.3 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa.

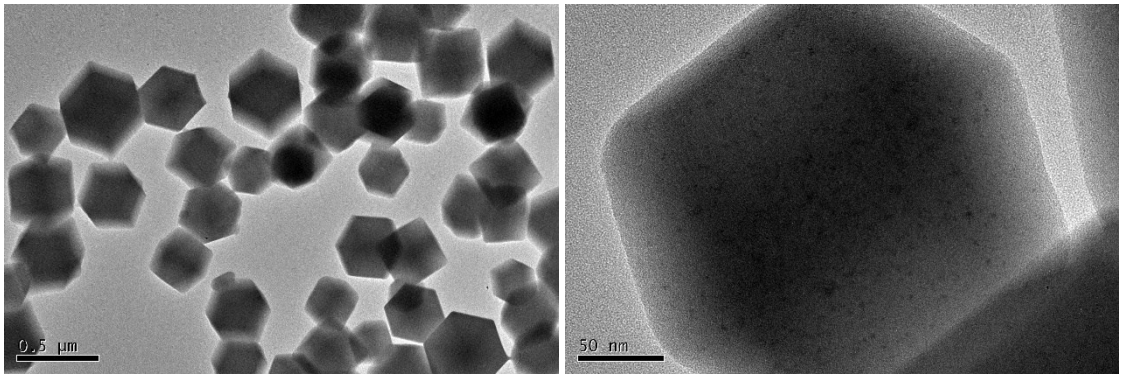


Fig. S7. TEM images of Pt-1.16@ZIF-8 after reaction.

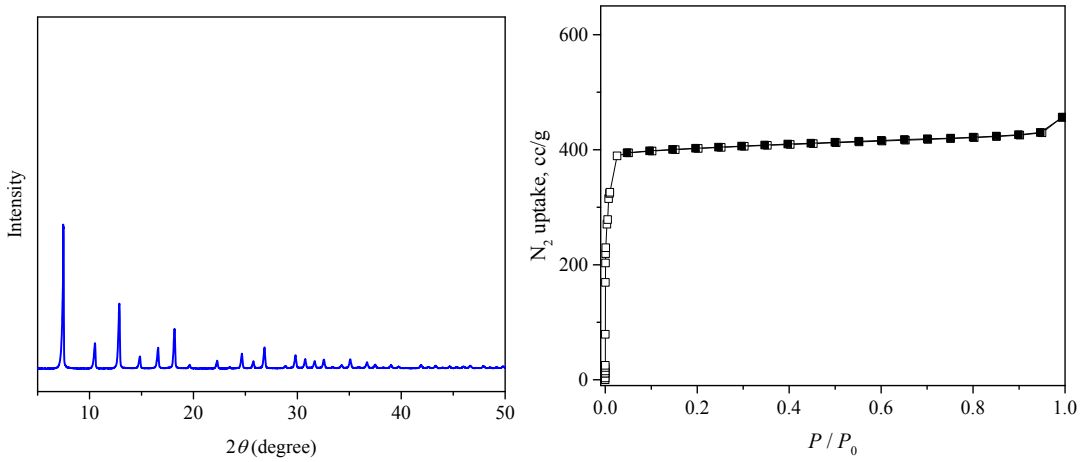


Fig. S8. XRD pattern (left) and N_2-sorption isotherms (right) of Pt-1.16@ZIF-8 after reaction.

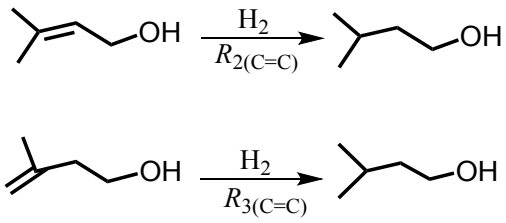
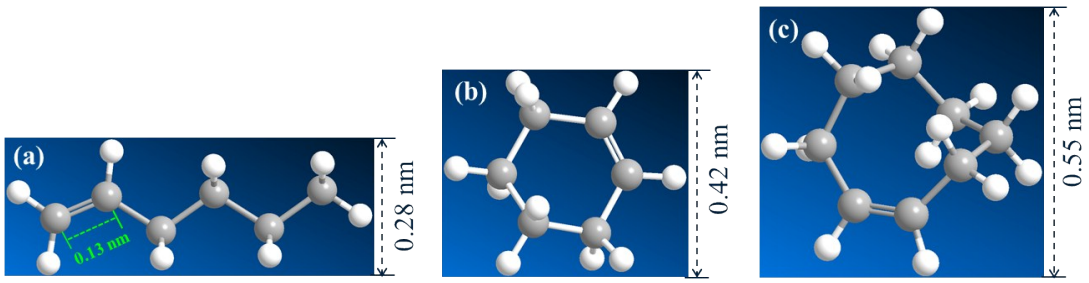


Fig. S9. Reaction pathway of the 3-methyl-2-butene-1-ol and 3-methyl-3-butene-1-ol hydrogenation.



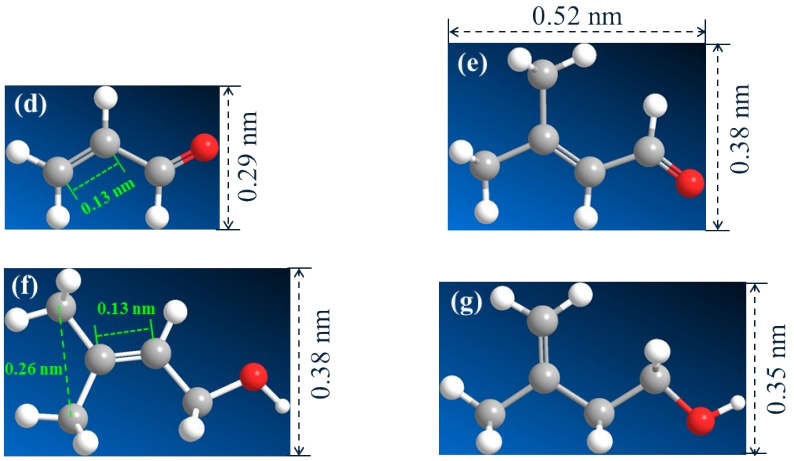


Fig. S10. Molecular structures of (a) 1-hexene, (b) cyclohexene, (c) cyclooctene, (d) acrolein, (e) 3-methylcrotonaldehyde, (f) 3-Methyl-2-butene-1-ol, and (g) 3-Methyl-3-butene-1-ol.
Color code: carbon- brown, hydrogen- white, oxygen- red.

Table S1. Hydrogenation rates of C=C ($R_{C=C}$) and C=O ($R_{C=O}$) over Pt/SiO_2, Pt/ZIF and Pt@ZIF-8 catalysts.

Catalysts	*t*, h	Con., %	$R_{C=C}$, h^{-1}	$R_{C=O}$, h^{-1}
Pt-0.23/SiO_2[a]	2	16.2	25.7	11.98
Pt-0.47/ZIF-8[b]	2	11.7	1.73	2.39
Pt-0.62@ZIF-8[b]	2	18.7	0.19	3.74
Pt-1.16@ZIF-8[b]	2	31.2	0.30	3.31

[a] Reaction conditions: 0.5 g catalyst, 0.5 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa.

[b] Reaction conditions: 1.2 g catalyst, 0.3 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa.

Table S2. Comparison of Pt@ZIF-8, Pt/ZIF-8 and Pt/SiO_2 in the hydrogenation of 3-Methyl-2-butene-1-ol (prenol) and 3-Methyl-3-butene-1-ol.

Catalysts	*t*, h	3-Methyl-2-butene-1-ol		3-Methyl-3-butene-1-ol	
		Con., %	$R_{2(C=C)}$, h^{-1}	Con., %	$R_{3(C=C)}$, h^{-1}
Pt-1.16@ZIF-8[a]	4	5.7	1.2	21.8	4.7
Pt-0.62@ZIF-8[a]	6	1.8	0.5	6.4	1.7
Pt-0.47/ZIF-8[a]	6	4.9	1.7	5.1	1.8
Pt-0.23/SiO_2[b]	1	17.9	155.9	14.3	124.2

[a] Reaction conditions: 0.2 g catalyst, 0.2 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa.

[b] Reaction conditions: 0.1 g catalyst, 0.2 g reactant dissolved in 100 mL cyclohexane, 80 °C and 3.0 MPa.