Electronic Supplementary Material

The synergic effects of highly selective bimetallic Pt-Pd/SAPO-41 catalysts for the *n*-hexadecane hydroisomerization

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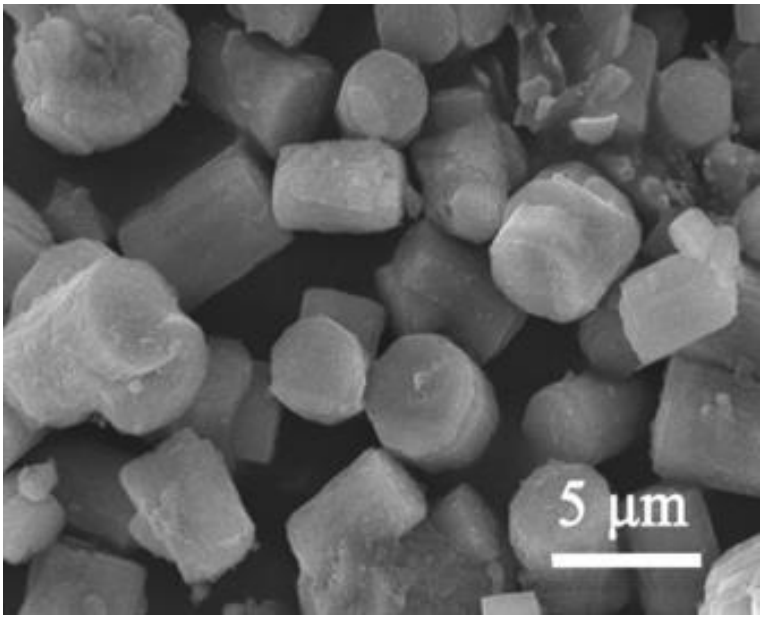

Fig. S1 SEM image of the SAPO-41 molecular sieve

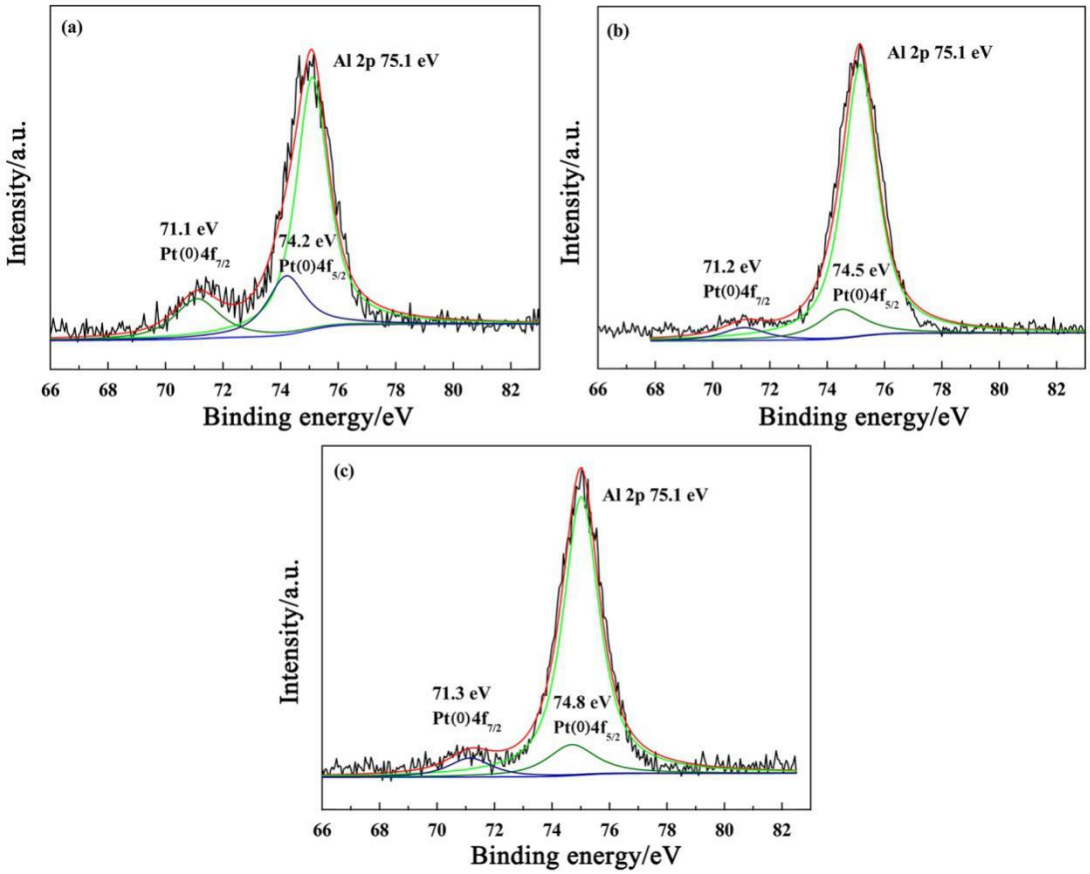

Fig. S2 XPS spectra of the Me/SAPO-41 bifunctional catalysts: (a) Pt/SAPO-41; (b) Pt*-Pd/SAPO-41 and (c) Pt-Pd/SAPO-41

Table S1 Physicochemical properties of the Pt-Pd/SAPO-41, 0.35Pt-0.15Pd/SAPO-41 and 0.15Pt-0.35Pd/SAPO-41 catalysts

Samples	Brønsted acid sites/(μmol·g^{-1})[a)]		C_{Me}/(μmol·g^{-1})[b)]	C_{Me}/C_{H^+}[c)]
	Strong	Total		
Pt-Pd/SAPO-41	18.6	35.1	17.7	0.50
0.35Pt-0.15Pd/SAPO-41	24.7	35.9	8.3	0.23
0.15Pt-0.35Pd/SAPO-41	26.2	41.6	7.7	0.19

a) Brønsted acid sites measured by Py-IR method.

b) The metal sites density (C_{Me}) calculated from metal dispersion by H_2 chemisorption method.

c) Ratio of C_{Me} to total Brønsted acid sites (C_{H^+}).

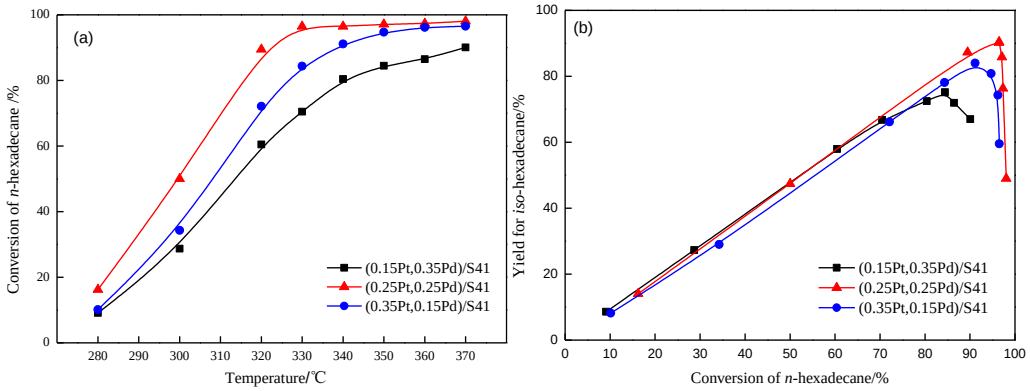

Fig. S3 The catalytic performances for *n*-hexadecane hydroisomerization over Pt-Pd/SAPO-41, 0.35Pt-0.15Pd/SAPO-41 and 0.15Pt-0.35Pd/SAPO-41 catalysts: (a) conversion of *n*-hexadecane and (b) yield of *iso*-hexadecane

Table S2 The catalytic performances over bifunctional catalysts with different metal loading in some reported references

Catalysts	Reactant	Total metal Loading/wt-%	Max yield of *iso*-alkane/%	Ref.
Pt/SAPO-31	*n*-heptane	0.5Pt	79.0	1
Pt/C-SAPO-11	*n*-dodecane	1.0Pt	84.0	2
Pt/SAPO-11	*n*-dodecane	0.5Pt	70.9	3
Pt/Fe-ZSM-22	*n*-dodecane	0.5Pt	78.8	4
Pt/Ca-H-ZSM-22	*n*-hexadecane	0.45Pt	77.8	5
Pt-Pd/H-beta	*n*-hexadecane	0.4Pt+0.4Pd	70.0	6
Pd*-Pt/Beta	*n*-hexane (65 wt-%), cyclohexane (20 wt-%) and *n*-heptane (15 wt-%)	0.5Pd+0.5Pt	34.9	7
Pt-Pd/H-Beta	*n*-hexane	0.5Pd+1.0Pt	82.0	8
Pd-Pt/ZrO_2-Al_2O_3-WO_3	*n*-hexane	1.0Pd+0.3Pt	61.3	9
Pt-Pd/WO_3-ZrO_2	*n*-decane	0.5Pt+0.27Pd	62.2	10
Pt-Pd/SAPO-41	*n*-hexadecane	0.25Pt+0.25Pd	89.4	this work

Table S3 Estimation of n_{as}, the average number of acid steps involved in the transformation of one molecule of *n*-hexadecane

Catalysts	Mono[a)]	Multi[b)]	Cracked[c)]	N_c[d)]	n_{as}[e)]
Pt/SAPO-41	0.60	0.20	0.20	2.90	1.99
Pd/SAPO-41	0.69	0.19	0.12	2.42	1.67
Pt*-Pd/SAPO-41	0.71	0.18	0.11	2.40	1.62
Pt-Pd/SAPO-41	0.81	0.12	0.07	2.04	1.39

a) Wt-% of Mono isomers = formed mono-branched *iso*-hexadecane / (*n*-hexadecane in – *n*-hexadecane out)

b) Wt-% of Multi isomers = formed multi-branched *iso*-hexadecane / (*n*-hexadecane in – *n*-hexadecane out)

c) Wt-% of cracked products = 1 – Wt-% of Mono isomers – Wt-% of Multi isomers

d) N_c = the number of cracked molecules (C_1-C_{15}) / the number of cracked hexadecane molecules

e) n_{as} = Mono × 1+Multi × 2.5+ Cracked × [4+ (N_C-2)/2]

The "formed mono-branched *iso*-hexadecane", "formed multi-branched *iso*-hexadecane", "*n*-hexadecane in" and "*n*-hexadecane out" are all quantified by quality, which were calculated based on the analysis results of GC spectra

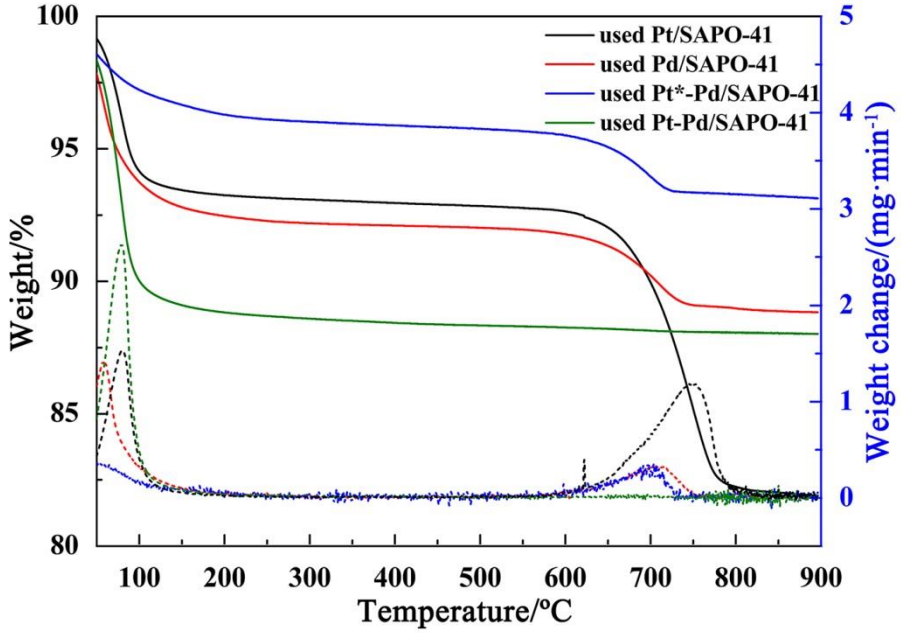

Fig. S4 TG and DTG curves of all used Me/SAPO-41 catalysts

Table S4 TG data and ΔC_{Me} value of all used Me/SAPO-41 catalysts

Catalysts	Weight loss/%		Temperature/ ℃		ΔC_{Me}/%[a)]
	Peak 1	Peak 2	Peak 1	Peak 2	
used Pt/SAPO-41	5.3	9.6	83	752	43.0
used Pd/SAPO-41	5.6	2.6	59	706	24.1
used Pt*-Pd/SAPO-41	2.3	2.1	63	694	18.7
used Pt-Pd/SAPO-41	9.1	0.5	81	696	7.9

a) The ΔC_{Me} value: the decrease percent of the metal site density of all used Me/SAPO-41 compared with the fresh catalysts.

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