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

Supporting Information

Insight into different performance of Pt/KL catalysts for *n*-alkane (C6-C8) aromatization: catalytic role of zeolite channels

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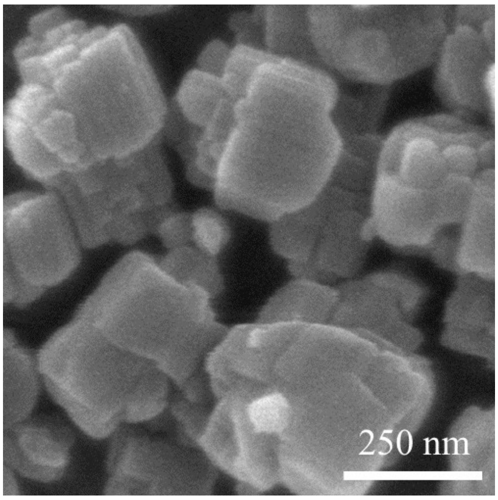

Fig. S1 The SEM image of KL zeolite

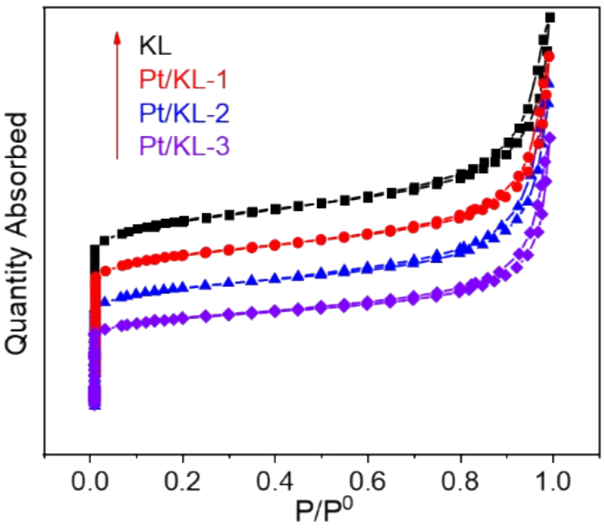

Fig. S2 N_2 adsorption-desorption isomers of KL zeolite and Pt/KL-x catalysts at 77 K

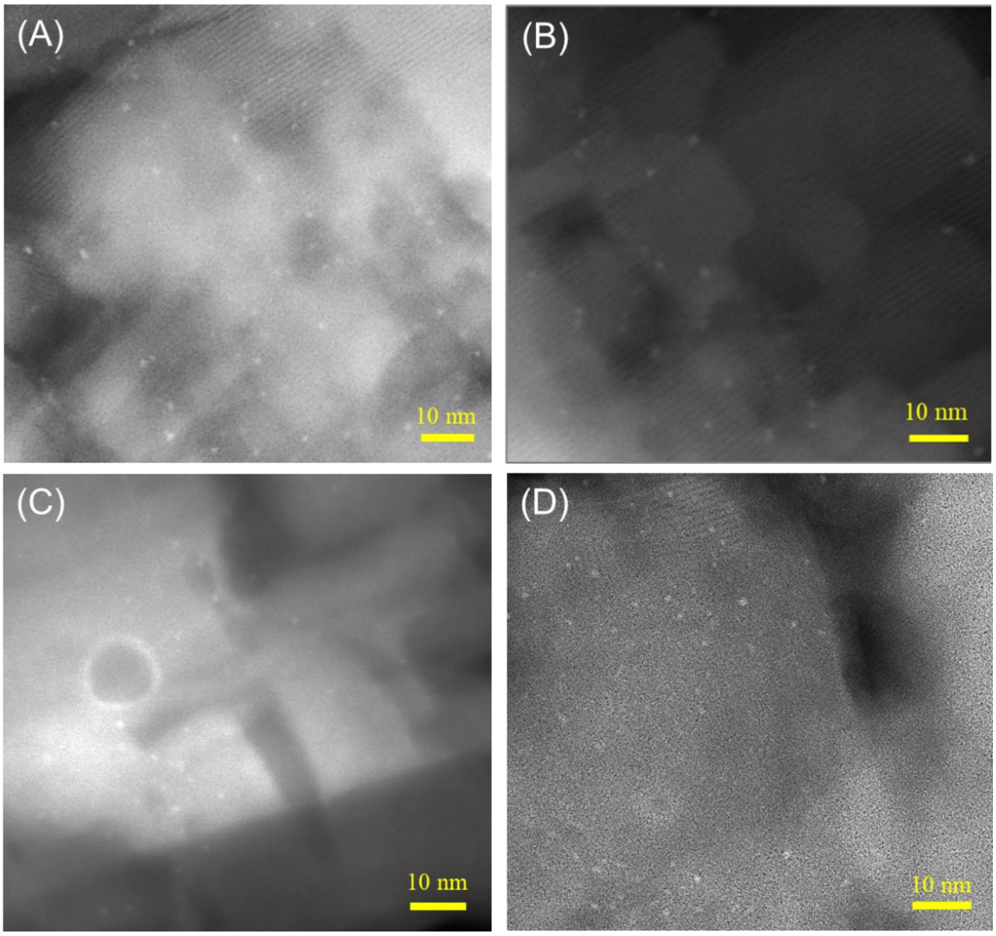

Fig. S3 HAADF-STEM of (A)-(B) Pt/KL-1 (C) Pt/KL-2 (D) Pt/KL-3 catalysts

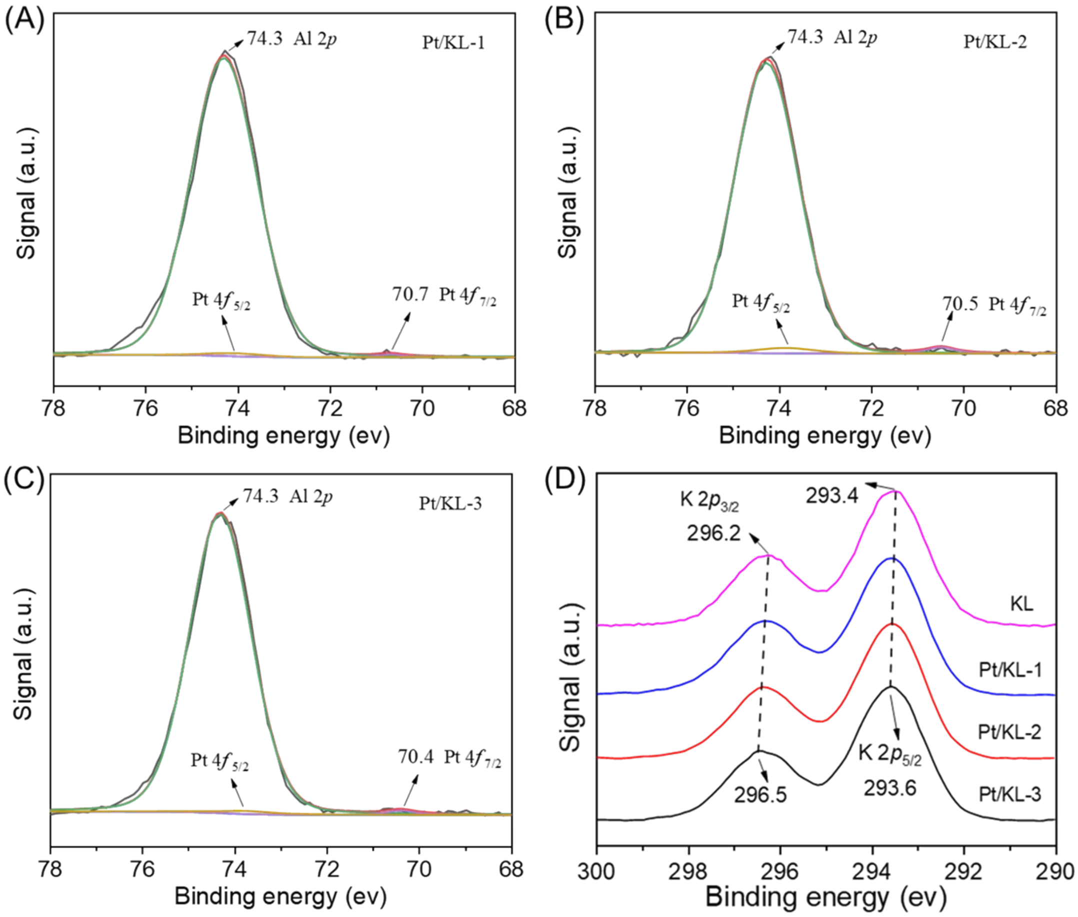

Fig. S4 The XPS spectra of Pt 4*f* for (A) Pt/KL-1 (B) Pt/KL-2 (C) Pt/KL-3 catalysts and (D) K 2*p* for Pt/KL-x catalysts

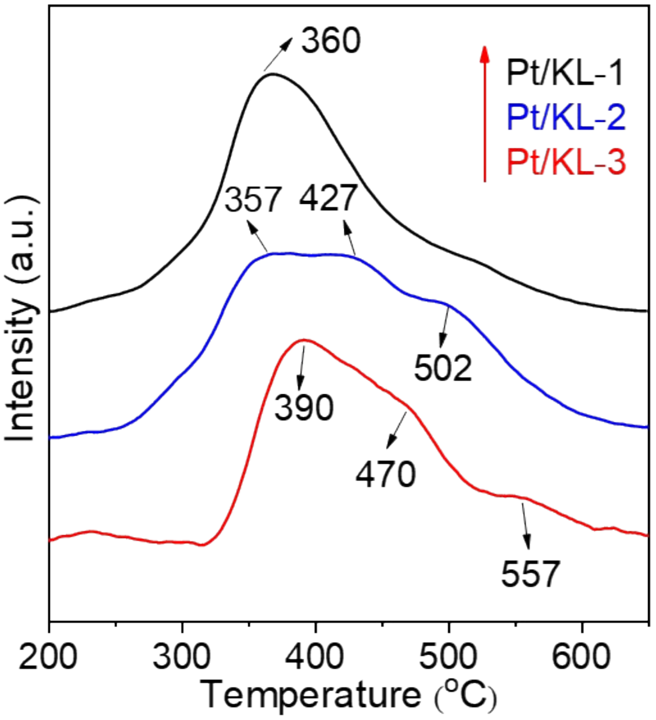

Fig. S5 The H_2-TPR profiles of Pt/KL-x catalysts

Table S1 Conversion and specific product selectivity of Pt/KL-3 catalyst for *n*-alkane aromatization (Reaction condition: T=450 °C; 0.1 MPa; H_2/*n*-alkane=6)

	Reactants		
	n-hexane	*n*-heptane	*n*-octane
Conversion / %	81.7	24.0	26.9
Selectivity / %			
total aromatics	83.2	48.0	41.0
benzene	83.2	6.7	2.3
toluene	-	41.3	4.8
C8 aromatics	-	-	33.9
C6=	0.7	0.6	0.1
C7=	-	19.0	0.3
C8=	-	-	24.1
C1-C4	3.5	5.2	6.2
C5-Cn [a]	12.6	27.2	28.3

[a] The value of n was 6, 7 and 8 when feed was *n*-hexane, *n*-heptane and *n*-octane, respectively

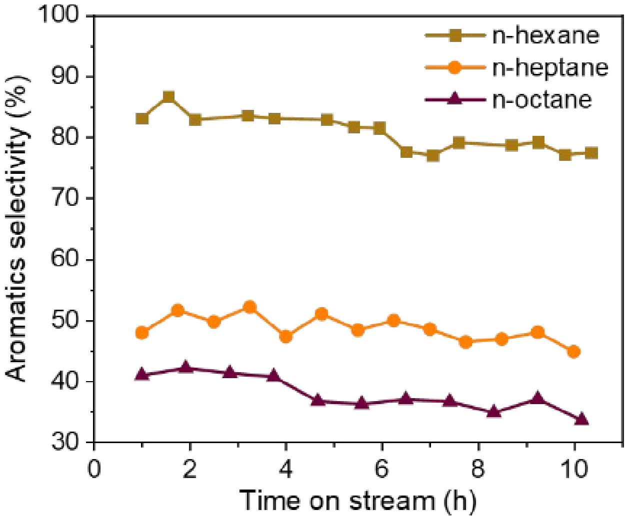

Fig. S6 Variation of aromatics selectivity in *n*-hexane, *n*-heptane and *n*-octane aromatization as a function of time on stream on Pt/KL-3 catalyst

(Reaction condition: T=450 ^{o}C; 0.1 MPa; H_2/*n*-alkane=6)

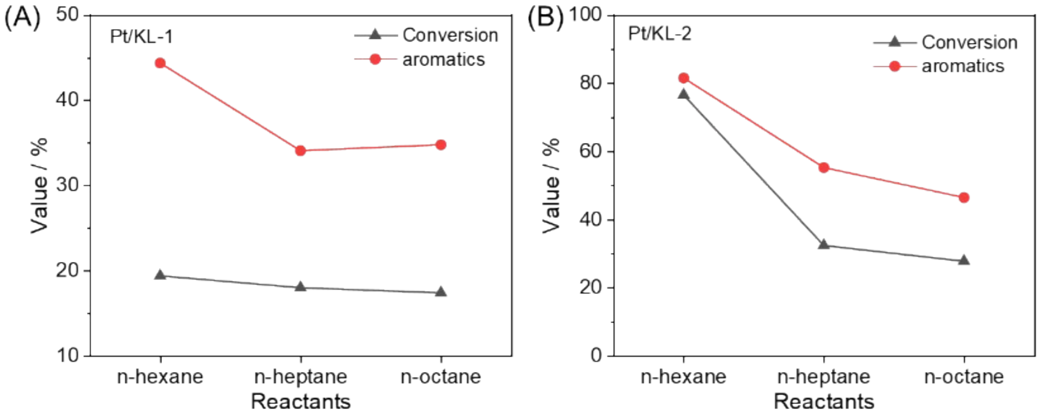

Fig. S7 The conversion and aromatics selectivity for *n*-hexane, *n*-heptane and *n*-octane aromatization over (a) Pt/KL-1 and (b) Pt/KL-2 catalysts

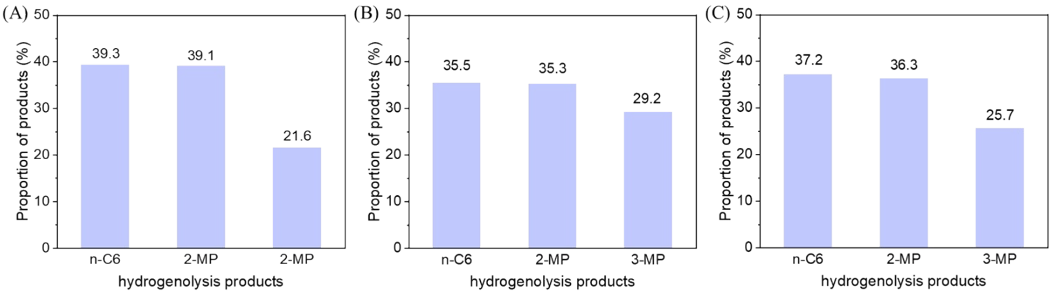

Fig. S8 The hydrogenolysis products distribution of methylcyclopentane on (A) Pt/KL-1 (B) Pt/KL-2 (C) Pt/KL-3 catalysts

The ring opening of methylcyclopentane was structure-sensitive reaction, and products distribution would be related to the size of Pt clusters and collimating effects of channels[1, 2]. For highlighting the effect of Pt clusters locations, methylcyclopentane hydrogenolysis was performed. The reaction conversion was controlled < 10%. The hydrogenolysis products distribution of methylcyclopentane on Pt/KL-x catalysts were shown in Fig. S8. For Pt/KL-1 catalyst (Fig. S8A), it could be seen that *n*-hexane, 2-methylpentane (2-MP) and 3-methylpentane (3-MP) accounted for 39.3%, 39.1% and 21.6% among total hydrogenolysis products, respectively. This indicated that the distribution was *n*-hexane: 2-MP: 3-MP = 1.82: 1.81: 1, which was similar to the statistical distribution (2: 2: 1)[3, 4]. The result suggested that Pt clusters of Pt/KL-1 catalyst were highly dispersed and mainly located outside zeolite channels. For Pt/KL-2 catalyst (Fig. S8B), the proportion of *n*-hexane, 2-MP and 3-MP were respectively 35.5%, 35.3% and 29.2% (*n*-hexane: 2-MP: 3-MP = 1.22: 1.21: 1), indicating increased selectivity of opening in the γ position[3]. This further confirmed that plentiful Pt clusters in Pt/KL-2 catalyst located inside zeolite channels, leading to evident collimating effects[2, 3]. While, the products distribution on Pt/KL-3 catalyst (1.45: 1.41: 1) was closer to statistical distribution (2: 2: 1), since parts of Pt clusters were again located at orifice in Pt/KL-3 catalyst. Above results further imply that the size of Pt clusters in these Pt/KL-x catalysts was similar and these clusters were not larger enough to fill pore. Therefore, the difference in catalytic performance of Pt/KL-x catalysts for *n*-alkane reforming might be related to the position of Pt clusters.

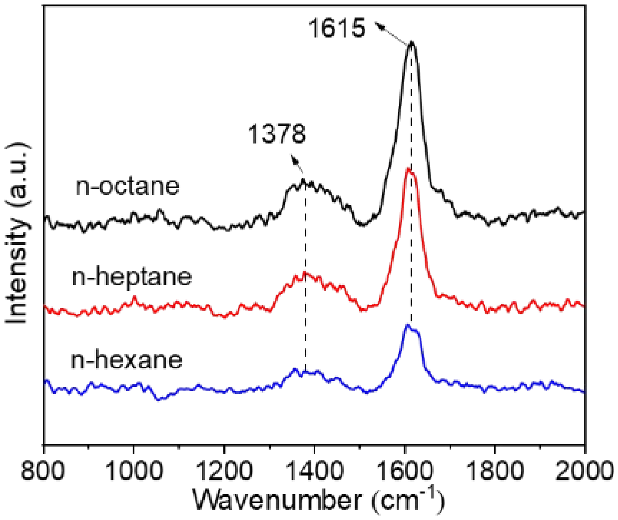

Fig. S9 UV-Raman spectra of spent Pt/KL-1 catalyst for *n*-alkane aromatization

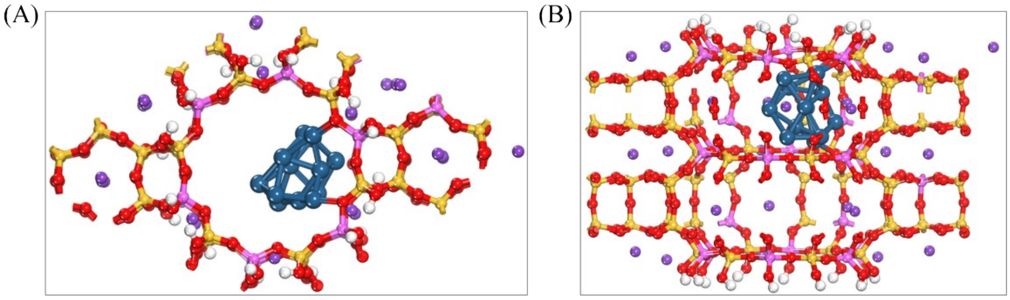

Fig. S10 The basal model of Pt/KL catalysts (A) projection viewed along [001]

(B) cartoon viewed [001]

Notes and references

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3 G. Jacobs, F. Ghadiali, A. Pisanu, A. Borgna, W. Alvarez and D. Resasco, *Appl. Catal. A.*, 1999, **188**, 79-98.

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