Electronic Supplementary Material

Propane dehydro-aromatization reaction over PtFe@S-1 coupling with Zn/ZSM-5 tandem catalysts: the role of Zn species

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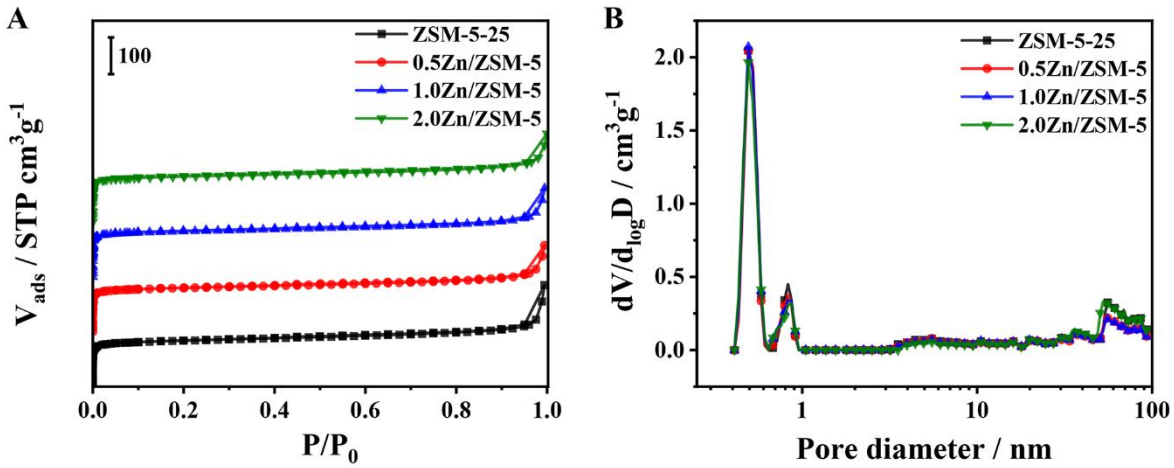

Fig. S1. The Ar adsorption-desorption (A) and pore distribution (B) results for ZSM-5-25 and different *x*Zn/ZSM-5 samples.

Table S1. The Ar adsorption-desorption and pore distribution results for ZSM-5-25 and different *x*Zn/ZSM-5 samples.

Catalysts	Surface Area (m^2g^{-1}) [a]	Micropore Volume (cm^3g^{-1}) [b]	Total Volume (cm^3g^{-1}) [c]
ZSM-5-25	434	0.16	0.35
0.5Zn/ZSM-5	417	0.16	0.31
1.0Zn/ZSM-5	432	0.16	0.32
2.0Zn/ZSM-5	416	0.15	0.34

[a] Calculated by BET model; [b] Calculated by SF model; [c] Estimated at $P/P_0 = 0.99$.

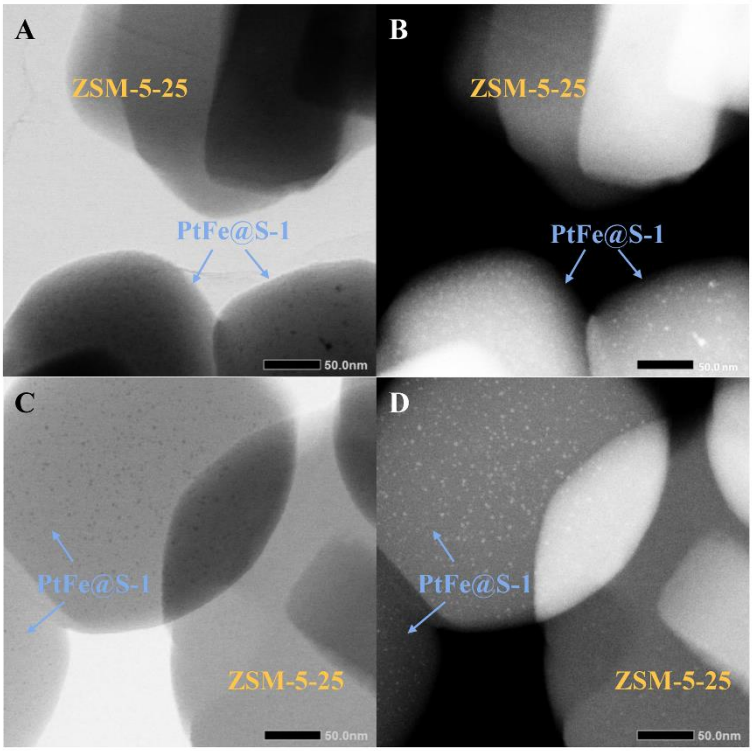

Fig. S2. The HR-TEM and HADDF-STEM images of powder mixed PtFe@S-1&ZSM-5-25 (A, B) and PtFeS-1&1.0Zn/ZSM-5 (C, D) catalyst after PDA reaction.

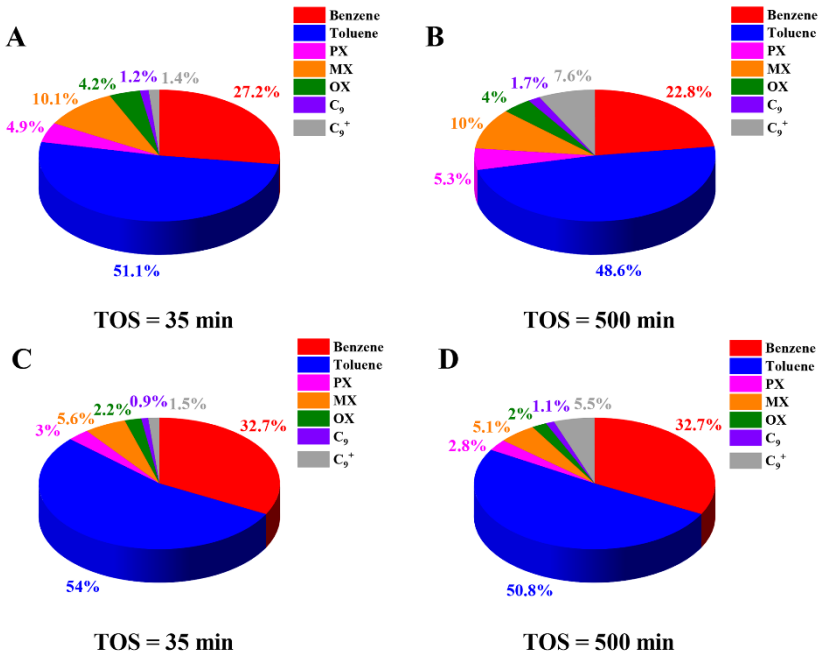

Fig. S3. The aromatics distribution of powder mixed PtFe@S-1&ZSM-5-25 (A, B) and PtFe@S-1&1.0Zn/ZSM-5 (C, D) with different time on stream (TOS= 35 or 500 min). Reaction conditions: T= 550 °C, ambient pressure, 0.30 g of PtFe@S-1&ZSM-5-25 or PtFe@S-1&1.0Zn/ZSM-5, C_3H_8/N_2= 5/35 mL/min

Table S2. The ICP results and acid properties for ZSM-5-25 and different *x*Zn/ZSM-5 samples.

Catalysts	Zn Content (%)[a]	Weak Acid Amount (μmol g^{-1})[b]	Strong Acid Amount (μmol g^{-1})[b]	Total Acid Amount (μmol g^{-1})[b]	Ratio of Brønsted/Lewis acid
ZSM-5-25	-	348	305	653	3.7
0.5Zn/ZSM-5	0.51	302	299	601	1.8
1.0Zn/ZSM-5	1.01	328	258	568	1.4
2.0Zn/ZSM-5	2.03	309	260	569	1.1

[a] Determined by ICP; [b] Calculated from NH_3-TPD; [c] Calculated from Py-IR.

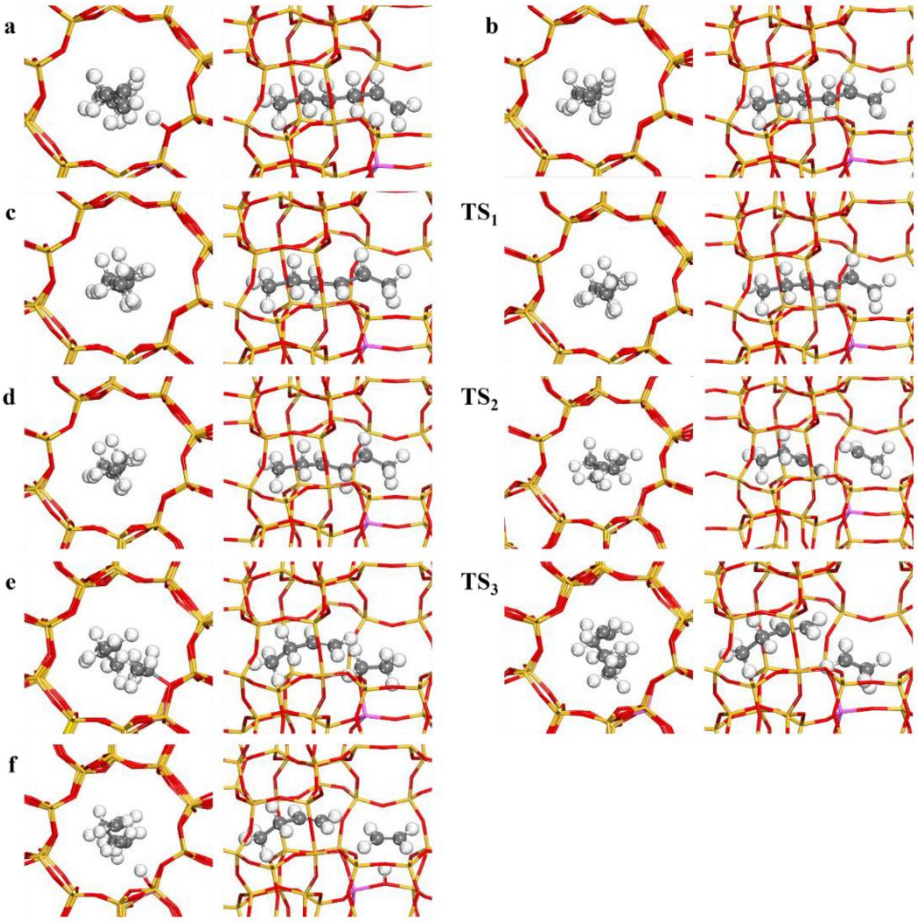

Fig. S4. Optimized structures involved in the 1-hexene cracking to C_2 and C_4 olefins on ZSM-5 (a-b-c-TS_1-d-TS_2-e-TS_3-f).

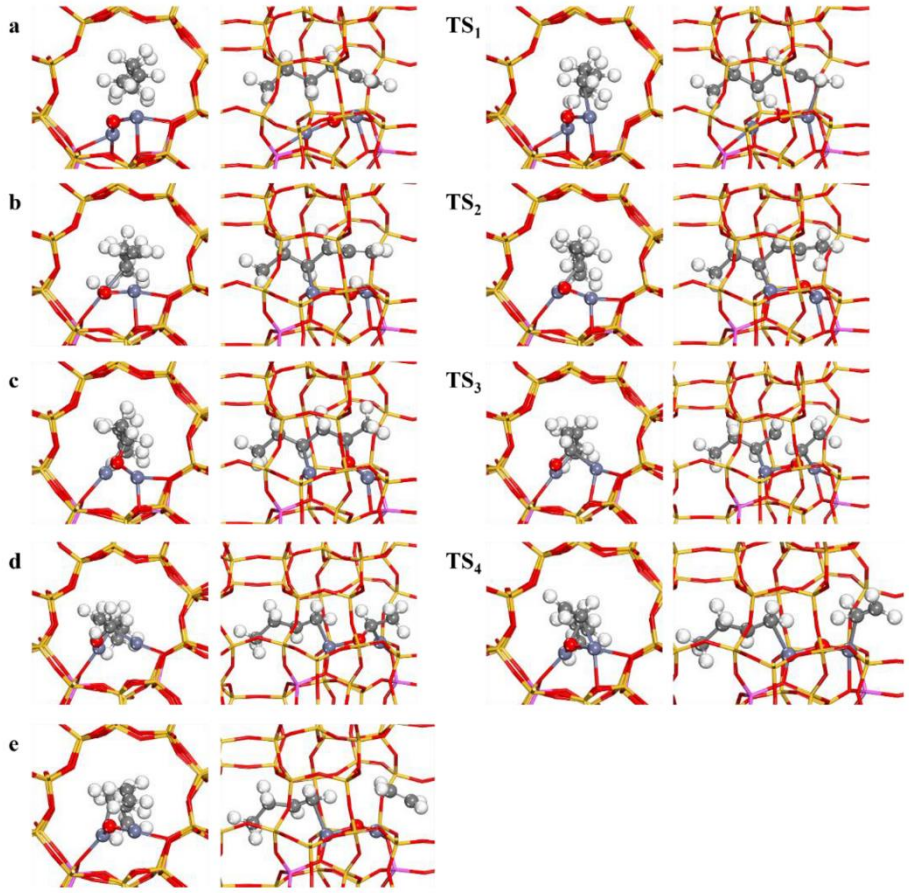

Fig. S5. Optimized structures involved in the 1-hexene cracking to C_2 and C_4 olefins on Zn/ZSM-5 (a-TS_1-b-TS_2-c-TS_3-d-TS_4-e).

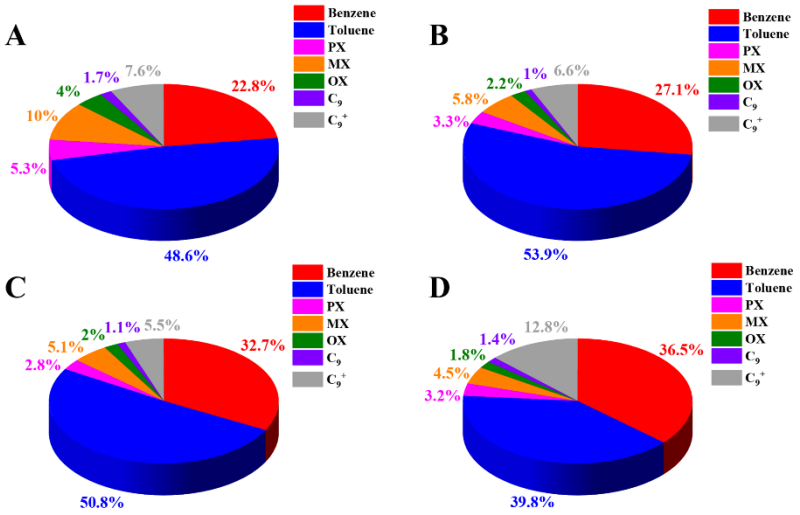

Fig. S6. The aromatics distribution of powder mixed PtFe@S-1&Zn/ZSM-5 with different amount of Zn in steady-state (TOS= 500 min). (A) ZSM-5; (B) 0.5Zn/ZSM-5; (C) 1.0Zn/ZSM-5; (D) 2.0Zn/ZSM-5. Reaction conditions: T= 550 °C, ambient pressure, 0.30 g of PtFe@S-1&*x*Zn/ZSM-5, C_3H_8/N_2= 5/35 mL/min