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Supporting Information

Bifunctional Intimacy and its Interplay with Metal-Acid Balance in Shaped Hydroisomerization Catalysts

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Bifunctional intimacy and its interplay with metal-acid balance in shaped hydroisomerization catalysts

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Figure S1: Average electron probe microanalysis profiles of AI (red), Si (purple), and Pt (blue) along the diameter of the extrudate for a) 0.11Pt/HUSY+Al₂O₃ and b) 0.25Pt/HUSY+Al₂O₃. Full ordinates scale: 100% for AI, 50% for Si, and a) 0.2 and b) 0.5% for Pt. Reproduced from ^[1].



Figure S2: Average electron probe microanalysis profiles of AI (green), Si (purple), and Pt (blue) along the diameter of the extrudate for a) 0.04Pt/ Al₂O₃+HUSY, b) 0.07Pt/ Al₂O₃+HUSY, and c) 0.18Pt/ Al₂O₃+HUSY.



n-Hexadecane hydroisomerization

Figure S3: First-order plot for the consumption of *n*-C₁₆ at 483 K (●), 488 K (■), and 498 K (▲) over Pt/HUSY+Al₂O₃ catalysts ^[1]. Symbols stand for experimental data and lines for fitting results. The reaction was carried out at 1.1 MPa total pressure and a molar H₂ to *n*-C₁₆ ratio of 10.



Figure S4: First-order plot for the consumption of *n*-C₁₆ at 483 K (◆), 488 K (■), and 498 K (▲) over Pt/Al₂O₃+HUSY catalysts. Symbols stand for experimental data and lines for fitting results. The reaction was carried out at 1.1 MPa total pressure and a molar H₂ to *n*-C₁₆ ratio of 10.



Figure S5: Monobranched (■) and multibranched (◆) C₁₆ isomers, and cracking (▲) products selectivity as function of conversion at 483 K (closed symbols), 488 K (cross symbols), and 498 K (open symbols), for a) 0.25Pt/(HUSY+Al₂O₃) ^[1] and b) 0.18Pt/Al₂O₃+HUSY.

Table S1: Apparent activation energy for n-hexadecane hydroconversion, assuming a 1st-order kinetics.

Catalyst	Activation energy (kJ mol ⁻¹)	
0.11Pt/HUSY+Al ₂ O ₃	191	
0.25Pt/HUSY+Al ₂ O ₃	196	
0.04Pt/Al ₂ O ₃ +HUSY	180	
0.07Pt/Al ₂ O ₃ +HUSY	182	
0.18Pt/Al ₂ O ₃ +HUSY	195	

Dual-function kinetic model

Table S2: Parameters for Y_{i-C16,max} (Eq. 1) determined by fitting catalytic descriptors results to the dual-function kinetic model ^[2].

Catalyst series	Υ (%)	ε (10³)
Pt/HUSY+Al ₂ O ₃	62.3	1.9
Pt/Al ₂ O ₃ +HUSY	58.3	1.8

References

- [1] P. S. F. Mendes, J. M. Silva, M. F. Ribeiro, A. Daudin, C. Bouchy, *J. Ind. Eng. Chem.* **2018**, *62*, 72-83.
- [2] P. S. F. Mendes, J. M. Silva, M. F. Ribeiro, P. Duchêne, A. Daudin, C. Bouchy, *AIChE J.* **2017**, 63, 2864-2875.