

Well-alloyed Pt-Sb/Si-Beta from Surface Organometallic Chemistry for Propane Dehydrogenation

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Table S1. Single crystal data of PtCl₂(SbPh₃)₂.

Empirical formula	C ₃₆ H ₃₀ Cl ₂ PtSb ₂
Formula weight	972.09
Temperature	299.82(19) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 33.4097(2) Å □ α = 90° b = 10.19390(10) Å □ β = 94.41° c = 20.57450(10) Å □ γ = 90°
Volume	6986.43(9) Å ³
Z	8
Density (calculated)	1.848 Mg/m ³
Absorption coefficient	21.085 mm ⁻¹
F(000)	3680
Crystal size	0.21 × 0.14 × 0.14 mm ³
Theta range for data collection	4.311 to 76.149°
Index ranges	-38 ≤ h ≤ 41, -12 ≤ k ≤ 11, -25 ≤ l ≤ 25
Reflections collected	37084
Independent reflections	13894 [R(int) = 0.0514]
Completeness to theta = 67.684°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.17180
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	13894/0/739
Goodness-of-fit on F ²	1.016
Final R indices [I > 2σ(I)]	R1 = 0.0439, wR2 = 0.1187
R indices (all data)	R1 = 0.0475, wR2 = 0.1218
Extinction coefficient	n/a
Largest diff. peak and hole	2.211 and -1.506 e.Å ⁻³

Table S2. Textural properties of Pt-Sb catalysts.

Catalysts	Pore Volume (cm ³ /g)	Pore Diameter (nm)
PtSb ₂ /Si-Beta	0.41	14.3
Sb ₂ /Pt/Si-Beta	0.41	13.5
Pt/Sb ₂ /Si-Beta	0.39	13.7
Pt/Si-Beta	0.39	13.8

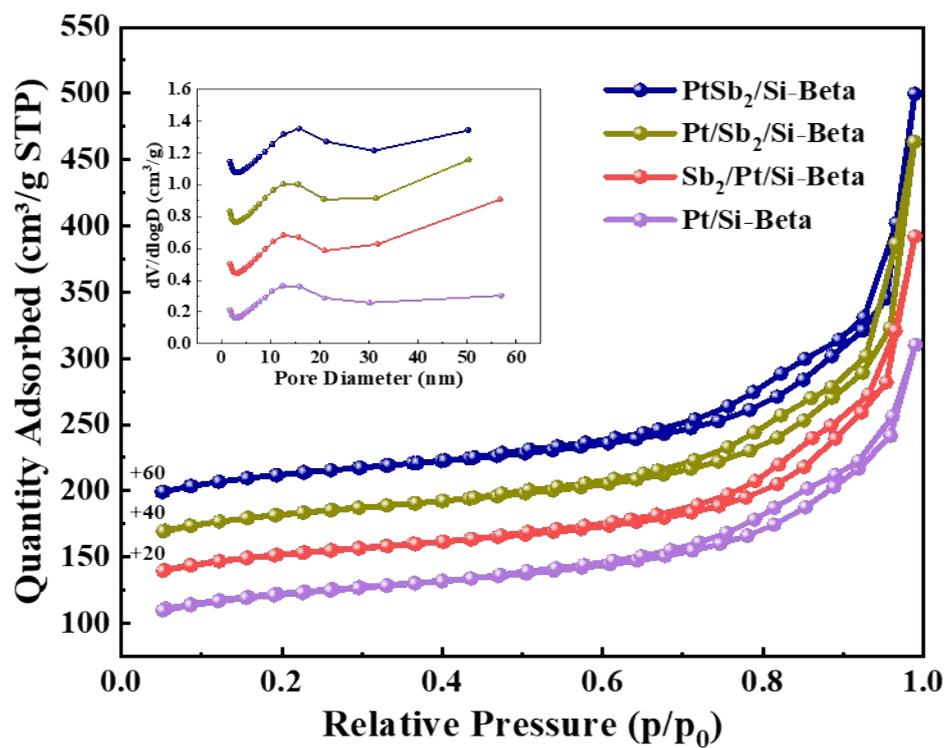


Figure S1. N₂ adsorption-desorption isotherms and pore diameter distributions of Pt/Si-Beta and Pt-Sb catalysts.

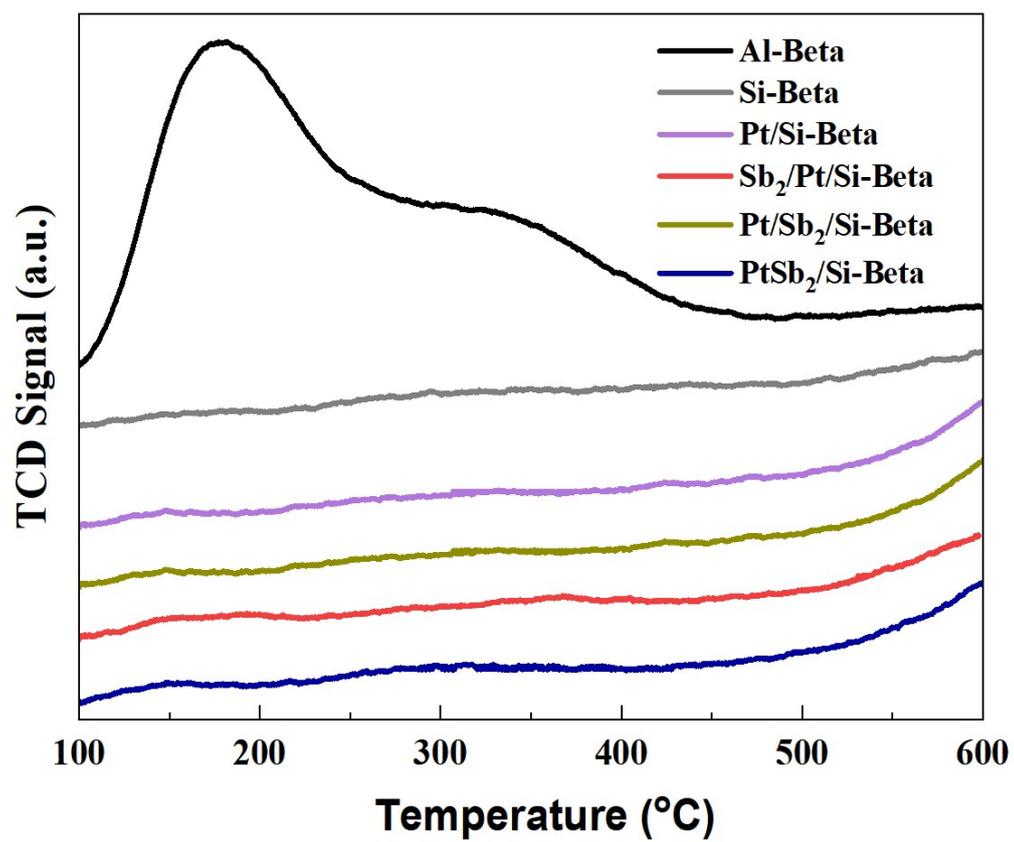


Figure S2. NH₃-TPD curves of Al-Beta, Si-Beta zeolite, Pt/Si-Beta and Pt-Sb catalysts.

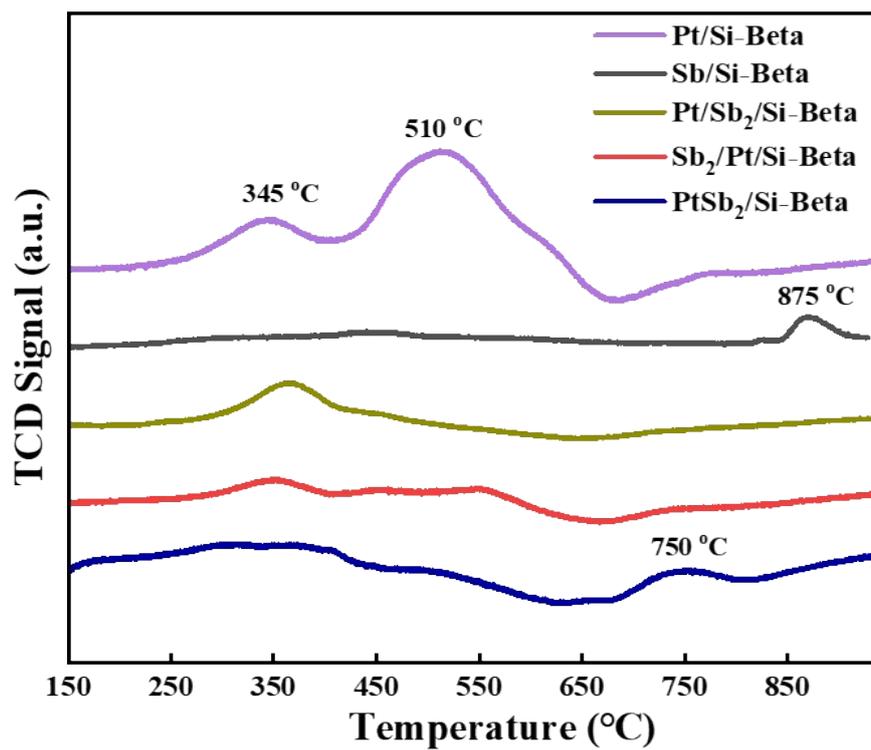


Figure S3. H₂-TPR curves of Pt/Si-Beta and Pt-Sb catalysts.