

Electronic Supplementary Material

Two-dimensional atomically thin Pt layers on MXenes: The role of electronic effects during catalytic dehydrogenation of ethane and propane

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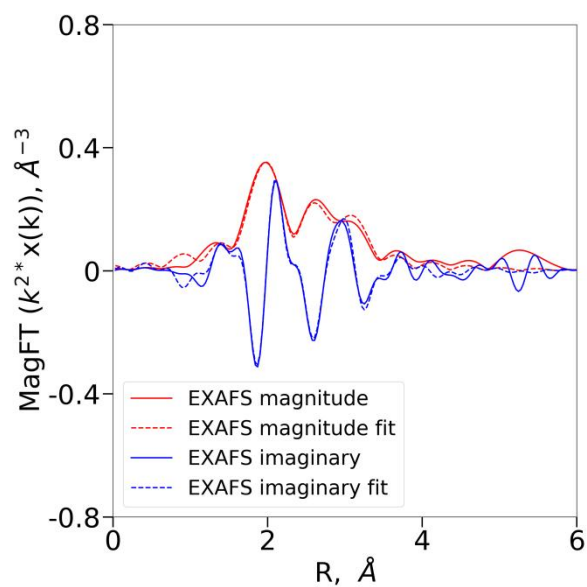


Figure S1. The magnitude (solid) and imaginary (dash) part of the Fourier transform of the k^2 weighted EXAFS and corresponding first shell fit for (a) Pt/Mo₂TiC₂T_x-750 °C.

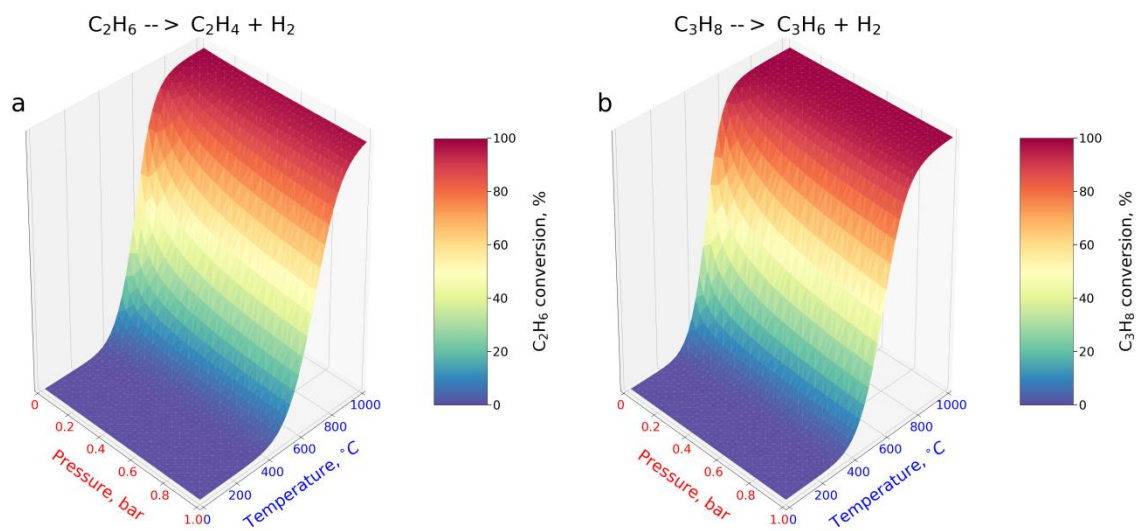


Figure S2. Effects of temperature and partial pressure on equilibrium conversion for (a) ethane dehydrogenation and (b) propane dehydrogenation.

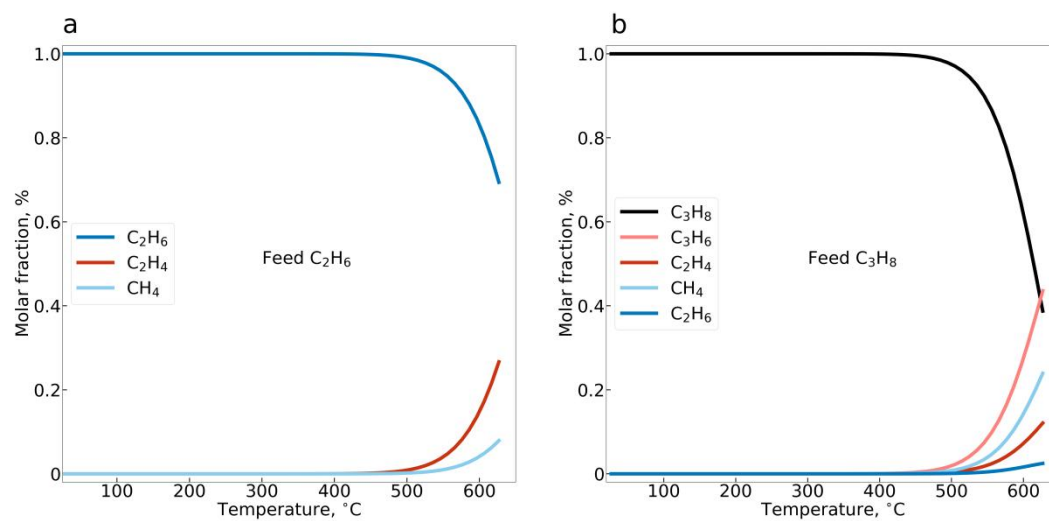


Figure S3. TPSR over 0.5% Pt/MXene for (a) ethane dehydrogenation at GHSV 57 h^{-1} and (b) propane dehydrogenation at GHSV 119 h^{-1} .

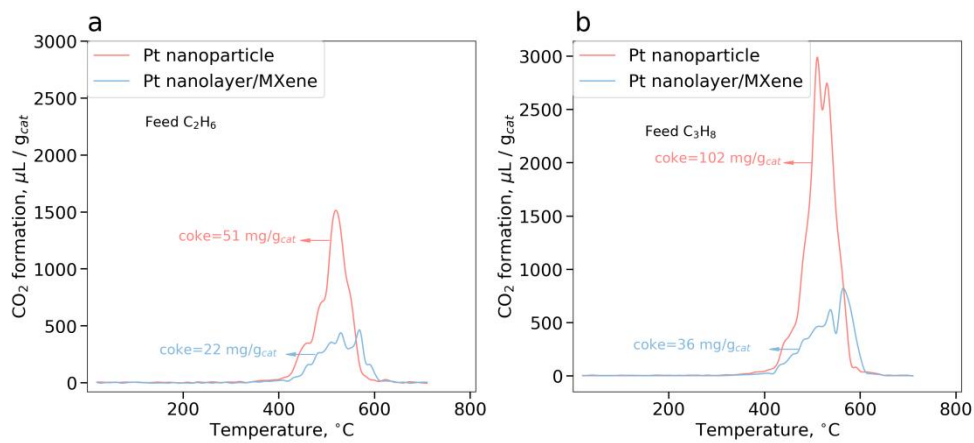


Figure S4. TPO profiles for 24-h spent 0.5% Pt/Mo₂TiC₂T_x (Pt nanolayer/MXene, blue curve) and 2-h spent 0.5% Pt/SiO₂ catalysts at 550 °C for (a) ethane dehydrogenation at GHSV 57 h⁻¹ and (b) propane dehydrogenation at GHSV 119 h⁻¹.

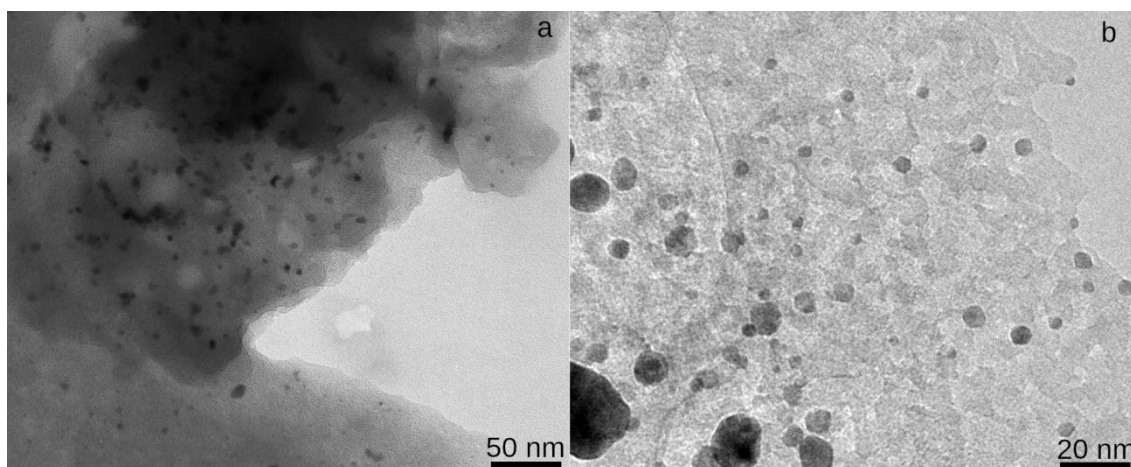


Figure S5. TEM scans for (a) fresh Pt/SiO₂ and (b) spent Pt/SiO₂ catalysts

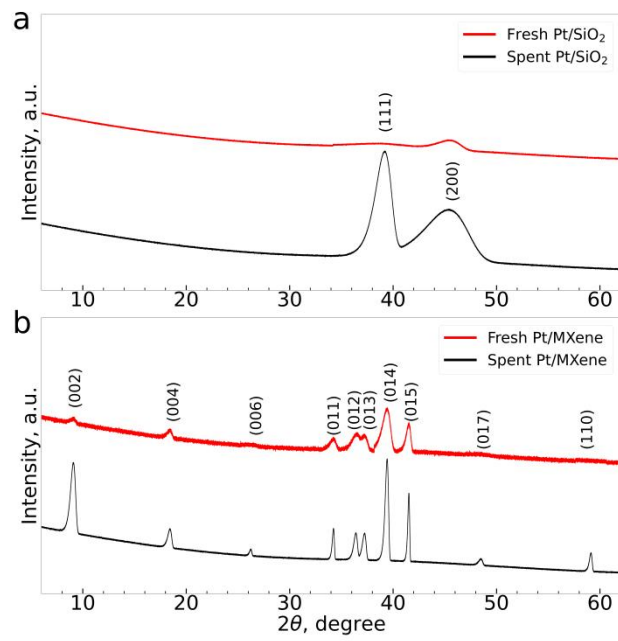


Figure S6. XRD patterns for (a) fresh and spent Pt/SiO₂ catalysts, and (b) fresh and spent Pt/MXene catalysts

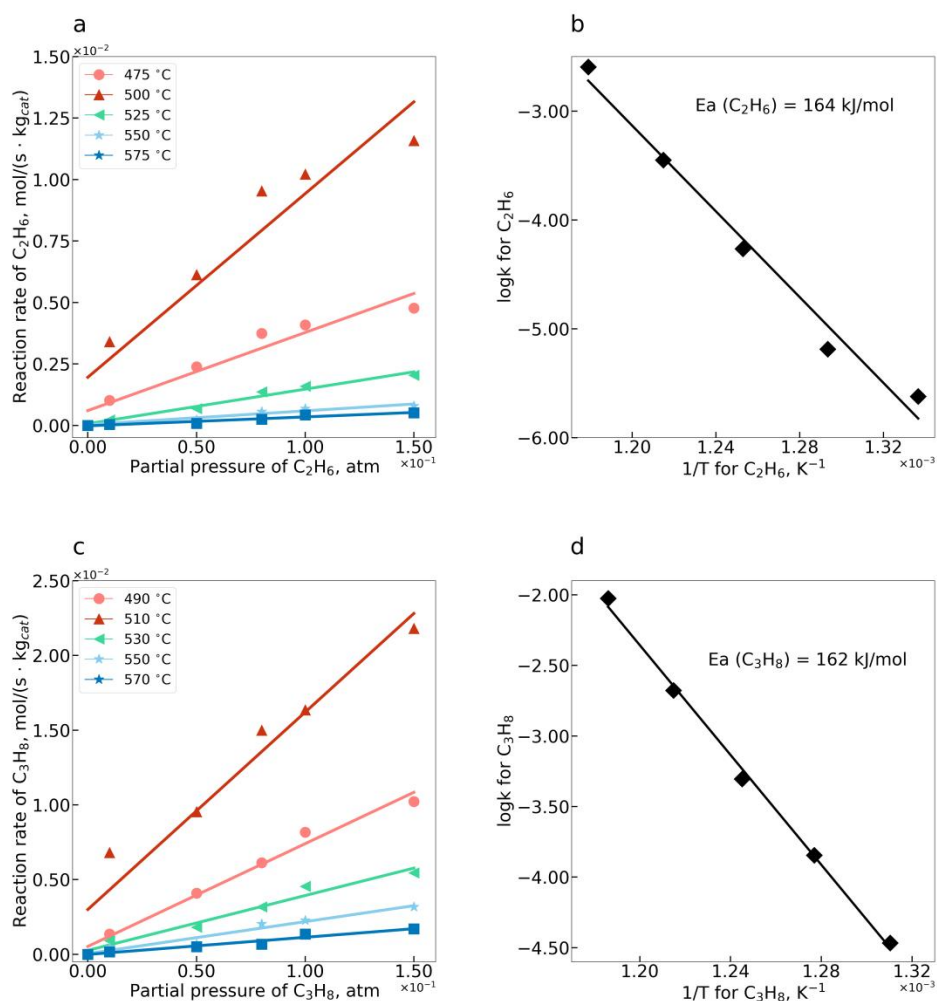


Figure S7. Investigations on ethane and propane kinetics, (a): fitting of ethane dehydrogenation, (b): Arrhenius plot for the rate constants of ethane dehydrogenation, (c): fitting of propane dehydrogenation, and (d): Arrhenius plot for the rate constants of propane dehydrogenation.

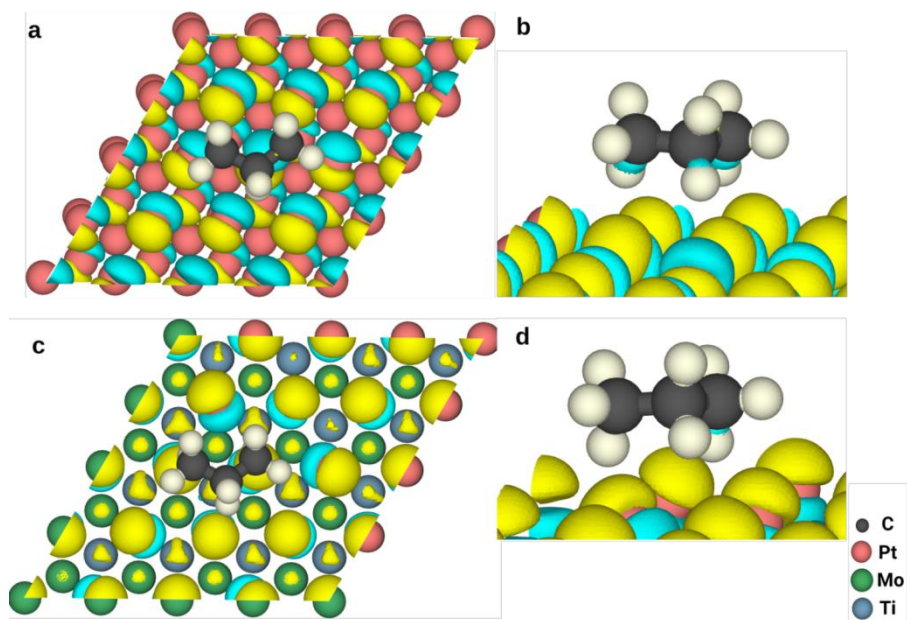


Figure S8. Charge Density Differences of Propane Dehydrogenation, (a) Pt(111) from the top view, (b) Pt(111) from the side view, (c) Pt/Mo₂TiC₂ from the top view, and (d) Pt/Mo₂TiC₂ from the side view. Blue color: negatively charged; Yellow color: positively charged

Table S1. Fitting results for the k^2 weighted EXAFS for Pt/Mo₂TiC₂T_x-R550 °C.

Sample	Scattering Pair	S_0^{2*}	CN	Bond Length (Å) #	σ^2 (Å ²) #	ΔE_0 (eV) #
Pt Foil	Pt-Pt	0.80	12	2.77	0.005	5.4
Pt/Mo ₂ TiC ₂ T _x R550C	Pt-Pt	0.80	7.9	2.75	0.014	4.0
	Pt-Mo		1.6	2.69	0.006	

* The S_0^2 for Pt/Mo₂TiC₂T_x samples are fixed at the value (0.80) obtained by fitting the Pt Foil

The average error in bond length is 0.01 Å, in σ^2 is 0.002 Å² and in ΔE_0 is 0.9 eV.

Table S2. Comparison of Pt dispersion measurements by H₂-O₂ titration, H₂ chemisorption and CO chemisorption

	H ₂ -O ₂ titration	H ₂ chemisorption	CO chemisorption
fresh Pt/SiO ₂	31%	33%	35%
spent Pt/SiO ₂	18%	16%	21%
fresh Pt/MXene	98%	95%	93%
spent Pt/MXene	98%	94%	94%