The comparison of two classes of bifunctional SBA-15 supported platinum-heteropolyacid catalysts for the isomerization of *n*-hexane

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Supporting Information for New Journal of Chemistry

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I. Catalysts characterization

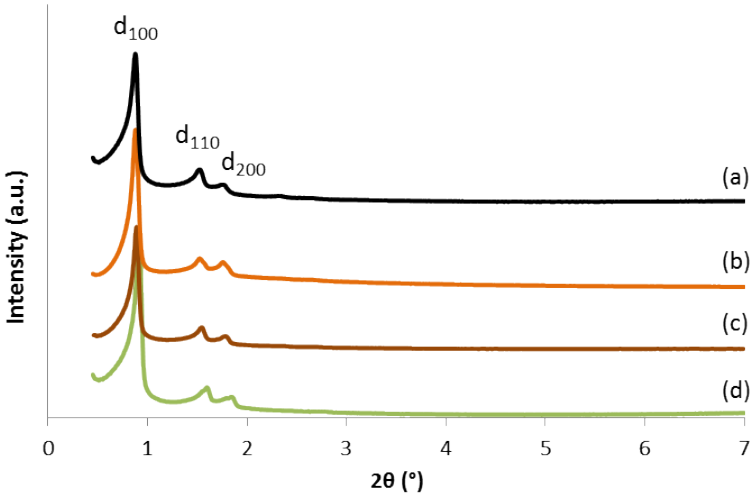


Figure S1. Low-angle XRD patterns of (a) pure SBA-15, (b) **Pt/SBA-15**, (c) **HSiW/Pt/SBA-15** and (d) **HSiW/SBA-15**.

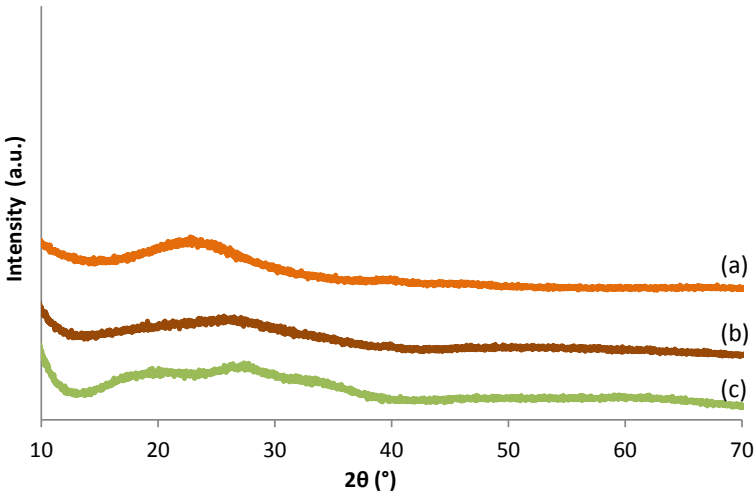


Figure S2. Wide-angle XRD patterns of (a) **Pt/SBA-15**, (b) **HSiW/Pt/SBA-15** and (c) **HSiW/SBA-15**.

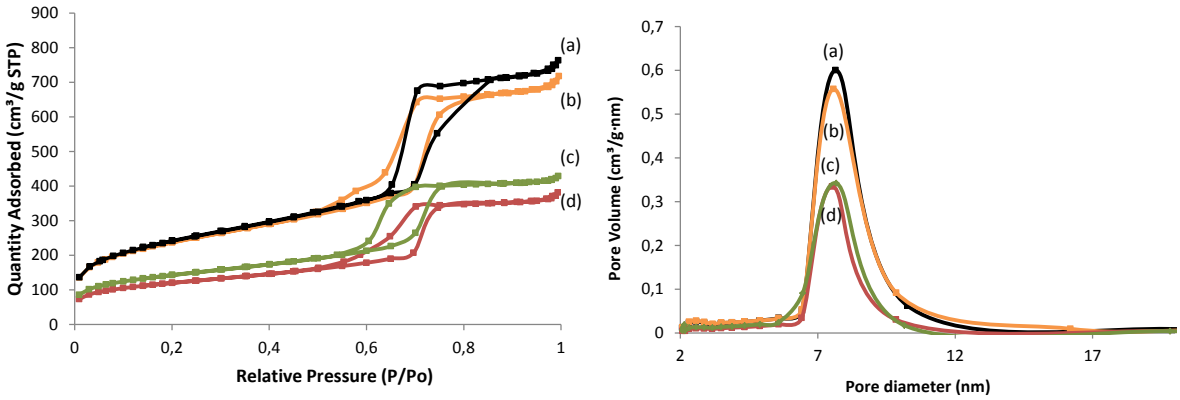


Figure S3. Nitrogen adsorption-desorption isotherms of (a) pure SBA-15, (b) **Pt/SBA-15**, (c) **HSiW/SBA-15** and (d) **HSiW/Pt/SBA-15**.

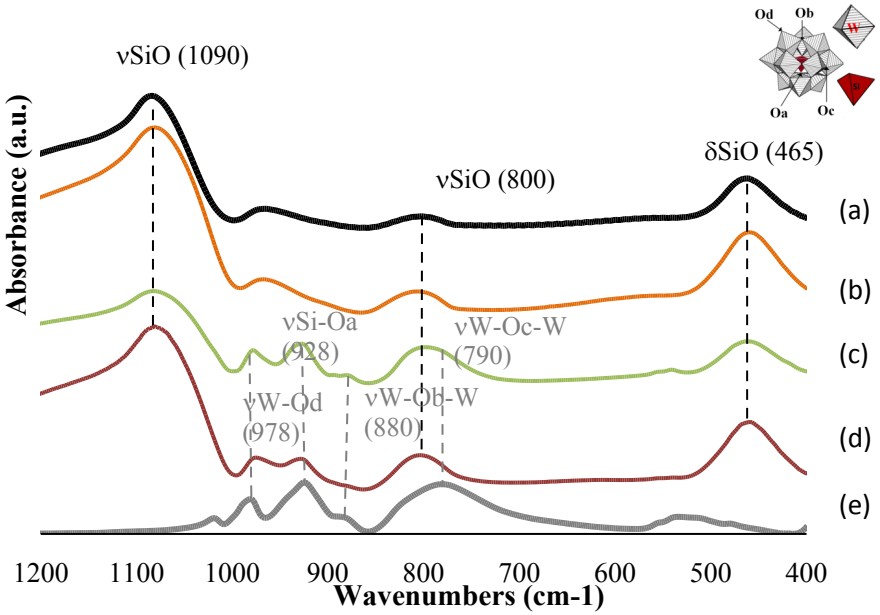


Figure S4. FT-IR spectra of (a) pure SBA-15, (b) **Pt/SBA-15**, (c) **HSiW/SBA-15**, (d) **HSiW/Pt/SBA-15** and (e) bulk $H_4SiW_{12}O_{40}$.

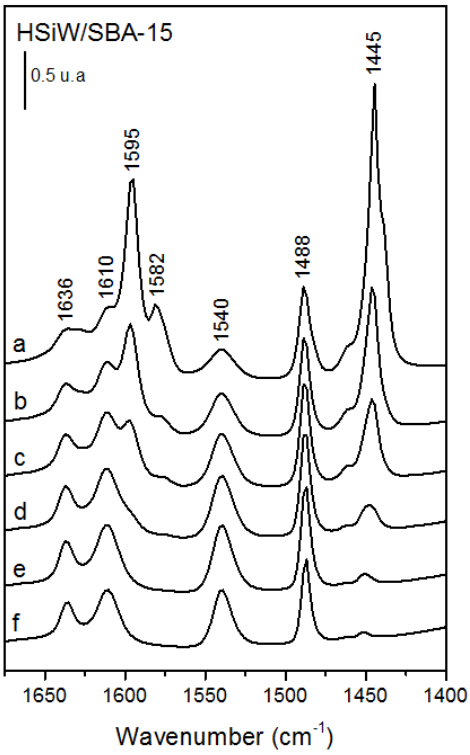


Figure S5. Infrared spectra of pyridine on **HSiW/SBA-15**, (a) adsorption at room temperature and as a function of the desorption temperature (b) room temperature, (c) 50 °C, (d) 100 °C, (e) 150 °C and (f) 200 °C.

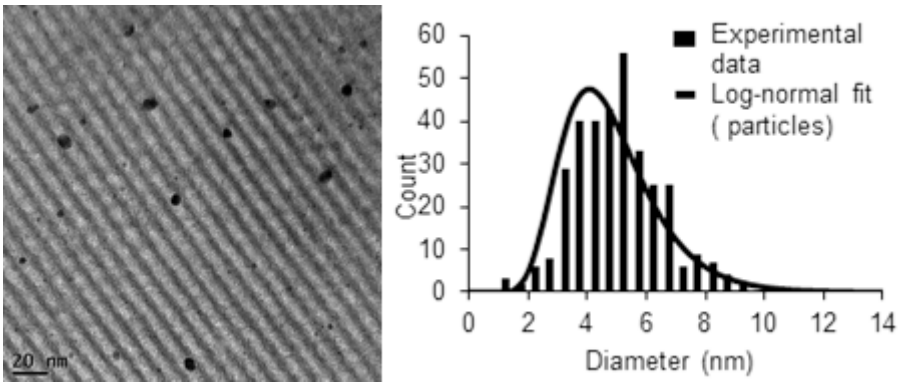


Figure S6. HRTEM image and particle size distribution of **Pt/SBA-15**. The number-average Pt particle size was obtained by counting 200 particles.

Table S1. Platinum atomic content of **Pt/SBA-15** determined by EDX (0.8 $\%_{wt}$ Pt ≅ 0.25 atom Pt per 100 atom Si).

Sampling	Si	Pt
1	100	0.30
2	100	0.36
3	100	0.21
4	100	0.24

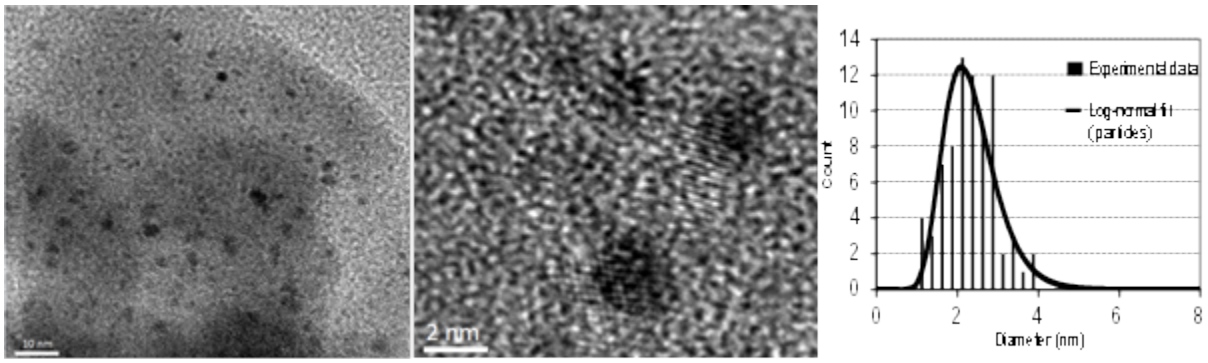
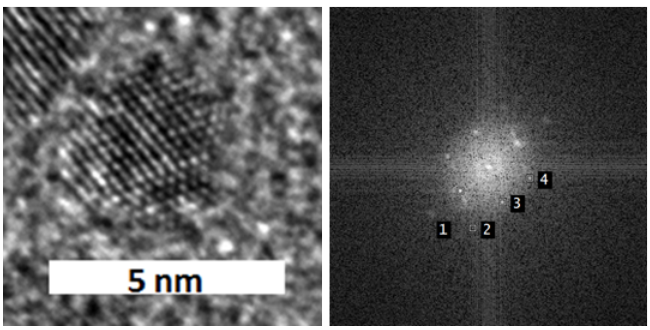


Figure S7. Representative HRTEM images and particle size distribution of **HSiW/Pt/SBA-15**. The number-average Pt particle size was obtained by counting 200 particles.



spot	hkl	d_{exp} nm	d_{theo} nm	Angle (exp) °	Angle (theo) °
1	200	0.2025	0.1962	0	0
2	111	0.2452	0.2265	53.9	54.7
3	-111	0.2328	0.2265	118.7	125.3
4	-311	0.1276	0.1183	153.7	154.8

Figure S8. HRTEM image and Fourier transform diffraction pattern of **Pt/SBA-15** and comparison between d spacing and angle with face-centered Pt cubic structure.

II. *n*-Hexane isomerization

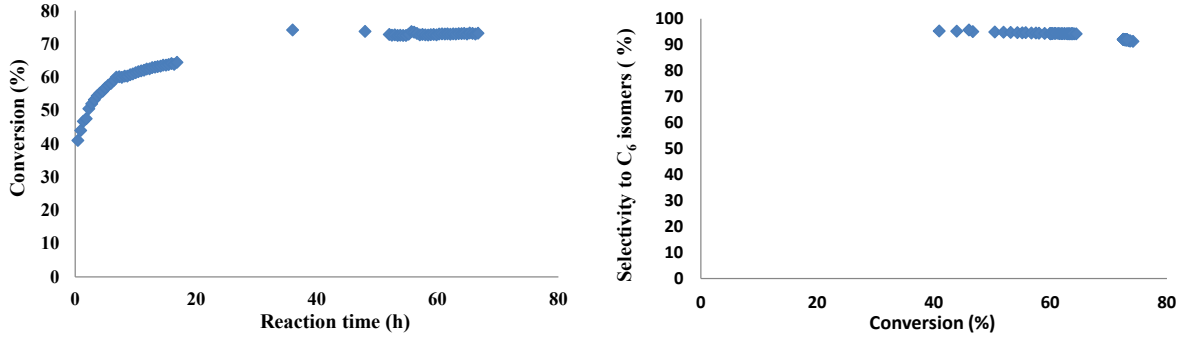


Figure S9. Conversion of *n*-hexane as a function of reaction time (left) and selectivity to C_6 isomers as a function of the conversion (right) for (**HSiW/SBA-15 + Pt/SBA-15**). Conditions: 1 bar, 200 °C, 5 mL.min^{-1} hydrogen flow, hexane/hydrogen ratio = 0.25, 1 g catalyst (0.5 g of each monofunctional catalyst).

Table S2. Apparent activation energy for bifunctional catalytic systems.

Catalyst	Activation energy [kJmol^{-1}]	R^2
HSiW/SBA-15 + Pt/SBA-15	66	0.99
HSiW/Pt/SBA-15	72	0.98

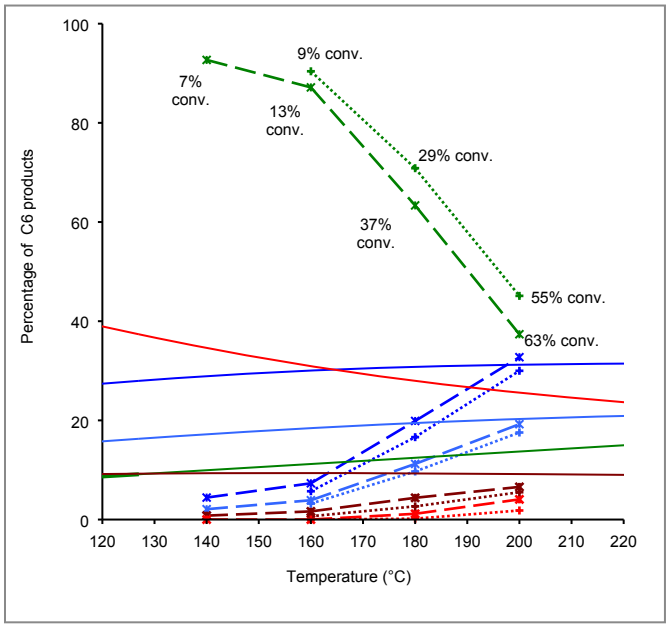


Figure S10. Evolution of the C_6 products as a function of temperature for the *multiphase* (**HSiW/SBA-15 + Pt/SBA-15**, dashed lines) and *monophase* (**HSiW/Pt/SBA-15**, dotted lines) bifunctional catalysts and comparison with the theoretical thermodynamic values (solid lines).[1] Products are color coded in the graph: *n*-hexane, green; 2-methyl pentane, dark blue; 3-methyl pentane, light blue; 2,2-dimethybutane, brown; 2,3-dimethybutane, red.

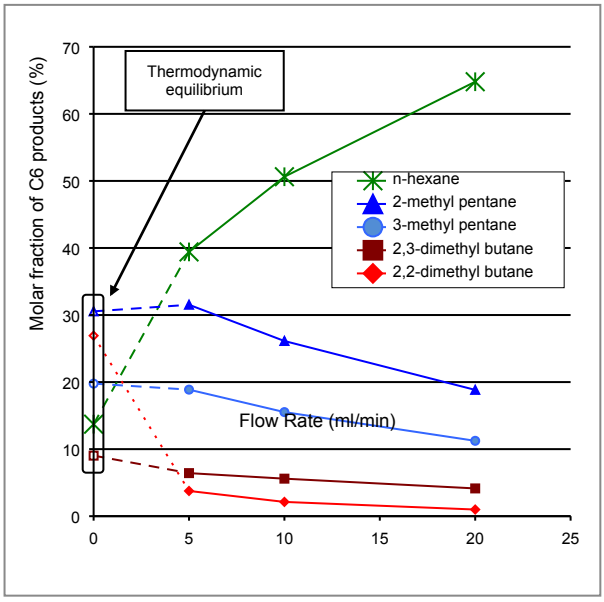


Figure S11. Evolution of the C_6 products as a function of flow rate for the *multiphase* bifunctional catalyst (**HSiW/SBA-15 + Pt/SBA-15**).

[1] R. A. Alberty, *Chem. Eng. Sci.*, 1987, **42**, 2325.

III. Catalysts characterization after catalysis

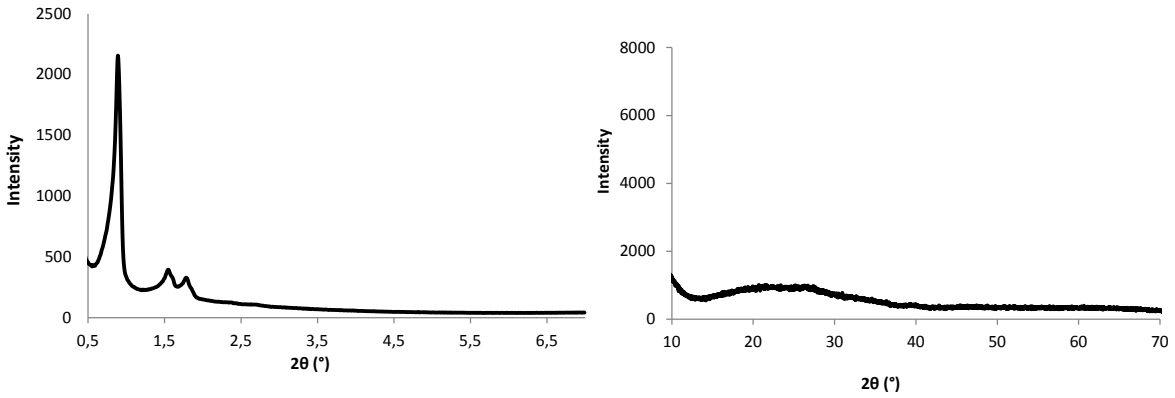


Figure S12. Low-angle (left) and wide-angle (right) XRD patterns of (**HSiW/SBA-15** + **Pt/SBA-15**) after catalysis (3 days on stream).

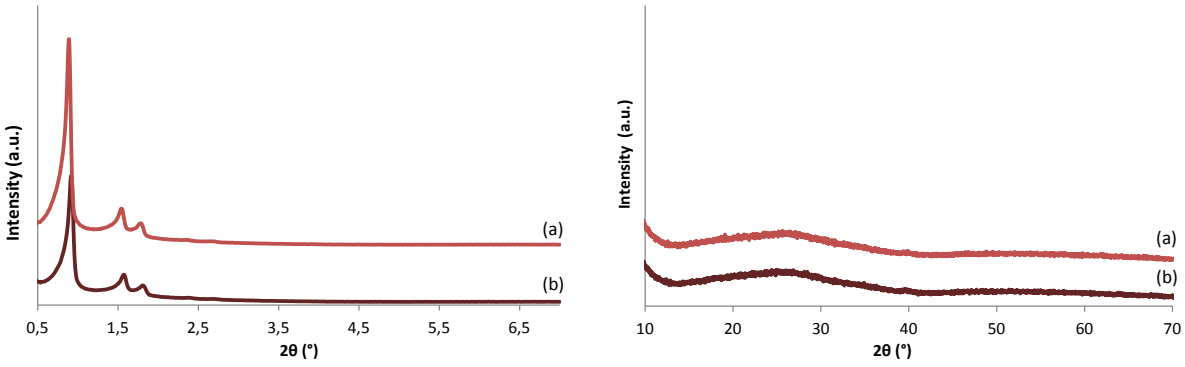


Figure S13. Low-angle (left) and wide-angle (right) XRD patterns of **HSiW/Pt/SBA-15** (a) before and (b) after catalysis (3 days on stream).

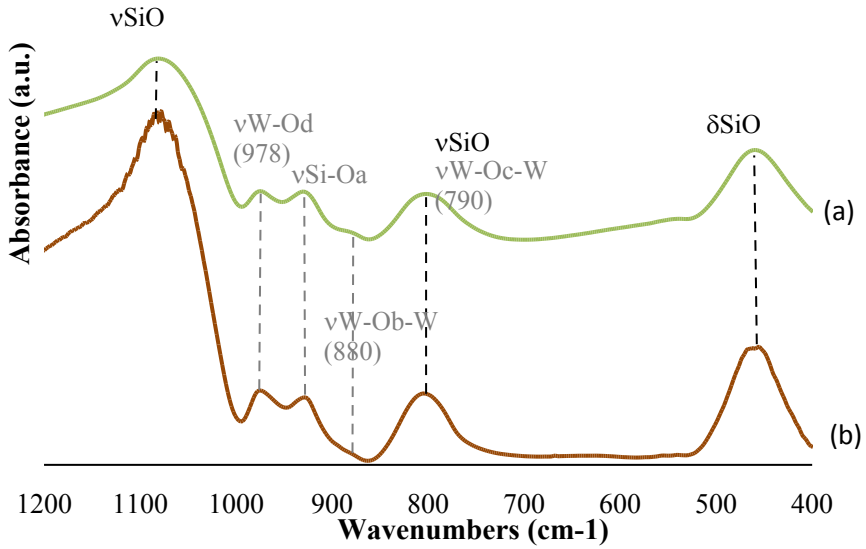


Figure S14. FT-IR spectra after catalysis (3 days on stream) of (a) (**HSiW/SBA-15** + **Pt/SBA-15**) and (b) **HSiW/Pt/SBA-15**.

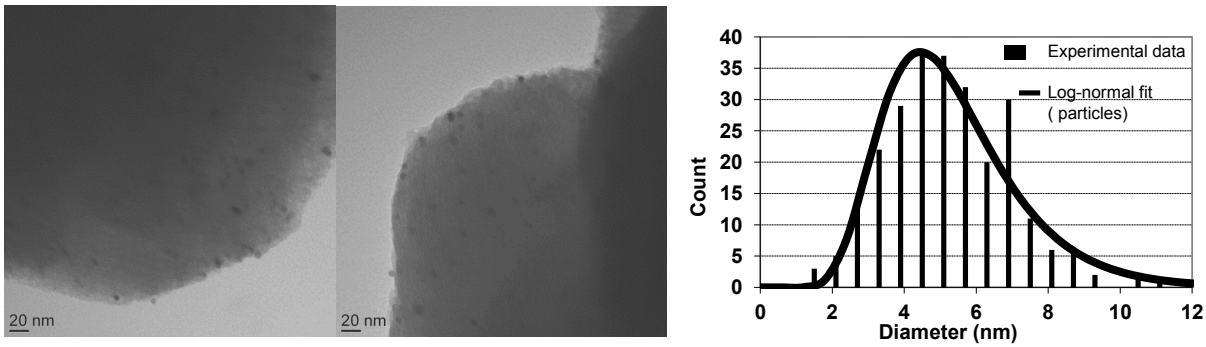


Figure S15. Representative HRTEM micrographs of (**HSiW/SBA-15** + **Pt/SBA-15**) after catalysis (3 days on stream) (Average Pt particles size = 5.3 ± 1.7 nm).

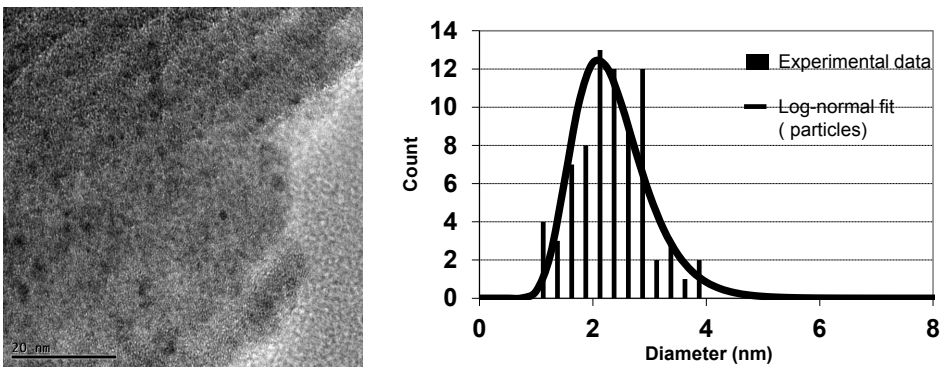


Figure S16. Representative HRTEM image of **HSiW/Pt/SBA-15** after catalysis (3 days on stream) (Average Pt particles size = 2.3 ± 0.6 nm).