

Supporting Information

Synergistic Catalysis of PdFe Bimetallic Nanoparticles Supported on SiO₂ for Hydrogenative Cleavage of C–N Bonds

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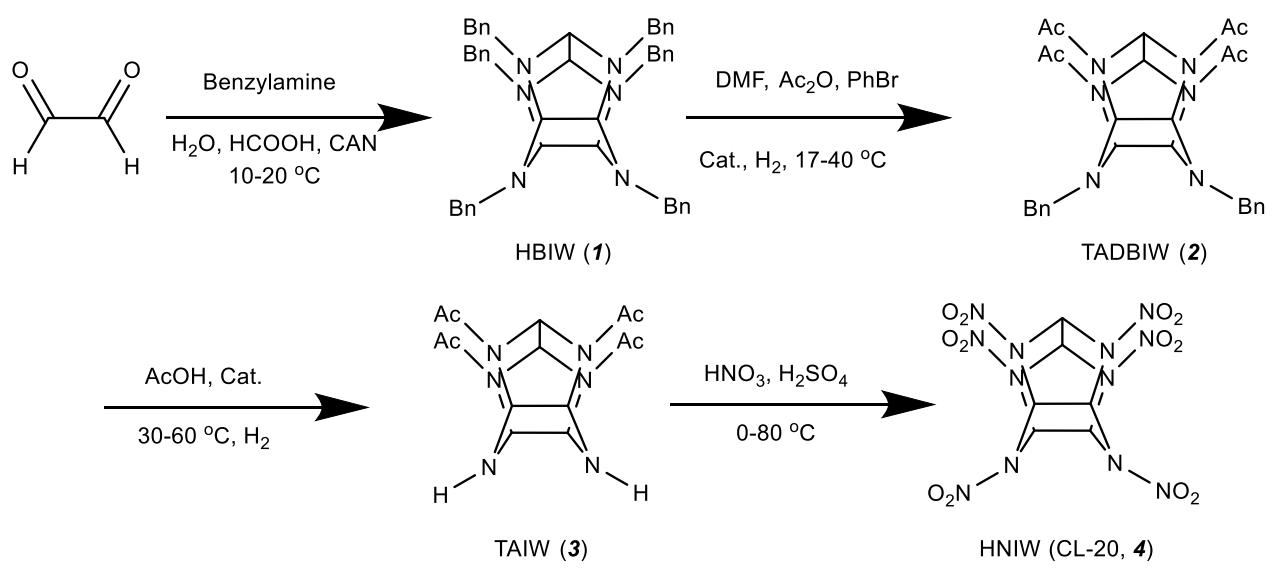
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Scheme S1. Synthesis of CL-20

Table S1. Surface state of the catalysts from XPS

sample	Pd ⁰		Pd ²⁺		ratio ^a	Fe ⁰	
	3d _{5/2}	3d _{3/2}	3d _{5/2}	3d _{3/2}		2p _{3/2}	2p _{1/2}
Pd₅/Si-CODP	335.6	340.9	336.7	342.0	2.4	-	-
Pd₅Fe_{0.5}/Si-CODP	335.7	341.0	336.9	342.0	2.4	711.6	724.9
Pd₅Fe₁/Si-CODP	335.6	340.9	336.8	342.1	2.4	712.5	725.8
Pd₅Fe₃/Si-CODP	335.6	340.9	336.7	342.0	1.1	712.2	725.5
Pd₅Fe₄/Si-CODP	335.9	341.2	337.0	342.3	1.5	712.2	725.5
Fe₁/Si-CODP	-	-	-	-	-	711.6	725.0
Pd₅/Fe₁/Si-DP	335.7	341.0	336.8	342.1	2.3	712.4	725.7
Fe₁/Pd₅/Si-DP	335.9	341.2	337.1	342.4	2.8	712.2	725.5

^a the ratio of Pd⁰ to Pd²⁺ based on the fitting peak areas.

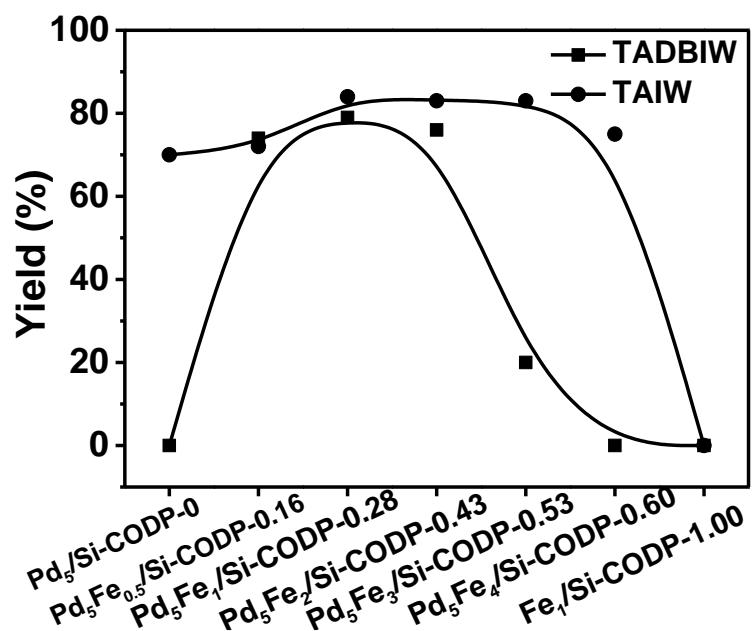


Figure S1. The yield of TADBIW (■) and TAIW (●) as a function of the ratio of Fe to bimetal over SiO₂ supports.

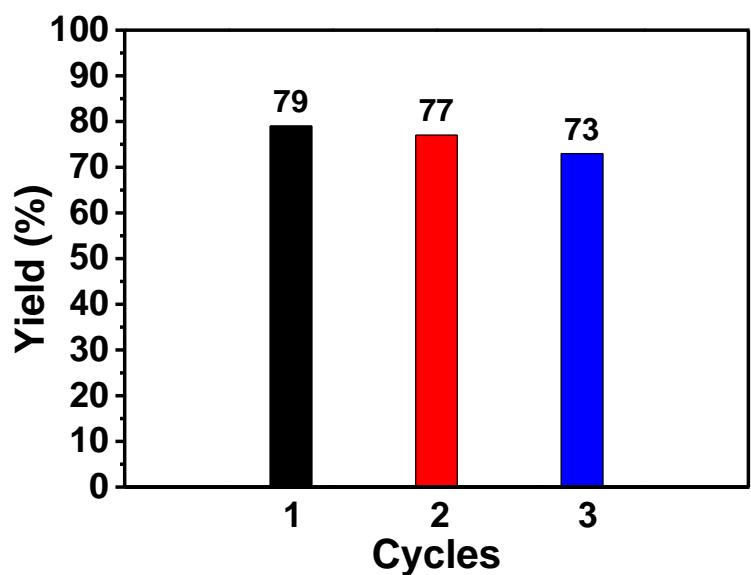


Figure S2. Recyclability of $\text{Pd}_x\text{Fe}_y/\text{SiO}_2$ -CODP for the hydrogenation debenzylation of HBIW. Run 1, black; run 2, red; run 3, blue.

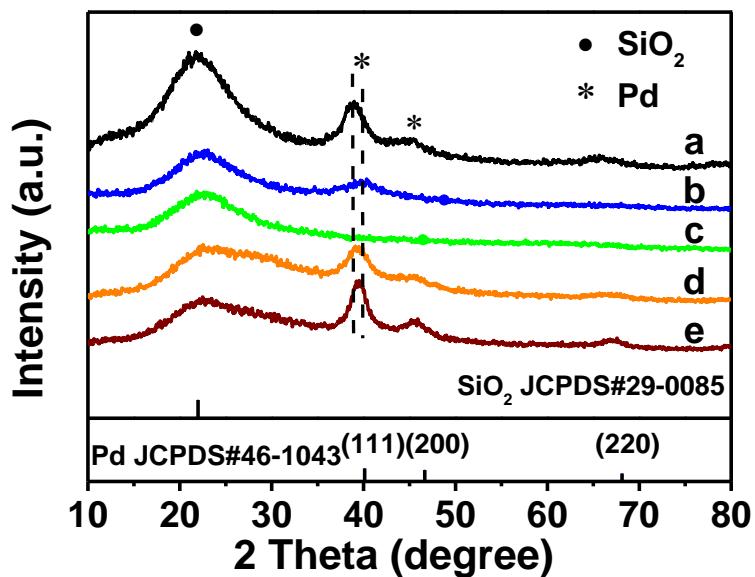


Figure S3. XRD patterns of the catalysts a. $\text{Pd}_5/\text{Si-CODP}$, b. $\text{Pd}_5\text{Fe}_1/\text{Si-CODP}$, c. $\text{Fe}_1/\text{Si-CODP}$, d. $\text{Pd}_5/\text{Fe}_1/\text{Si-DP}$, e. $\text{Fe}_1/\text{Pd}_5/\text{Si-DP}$.

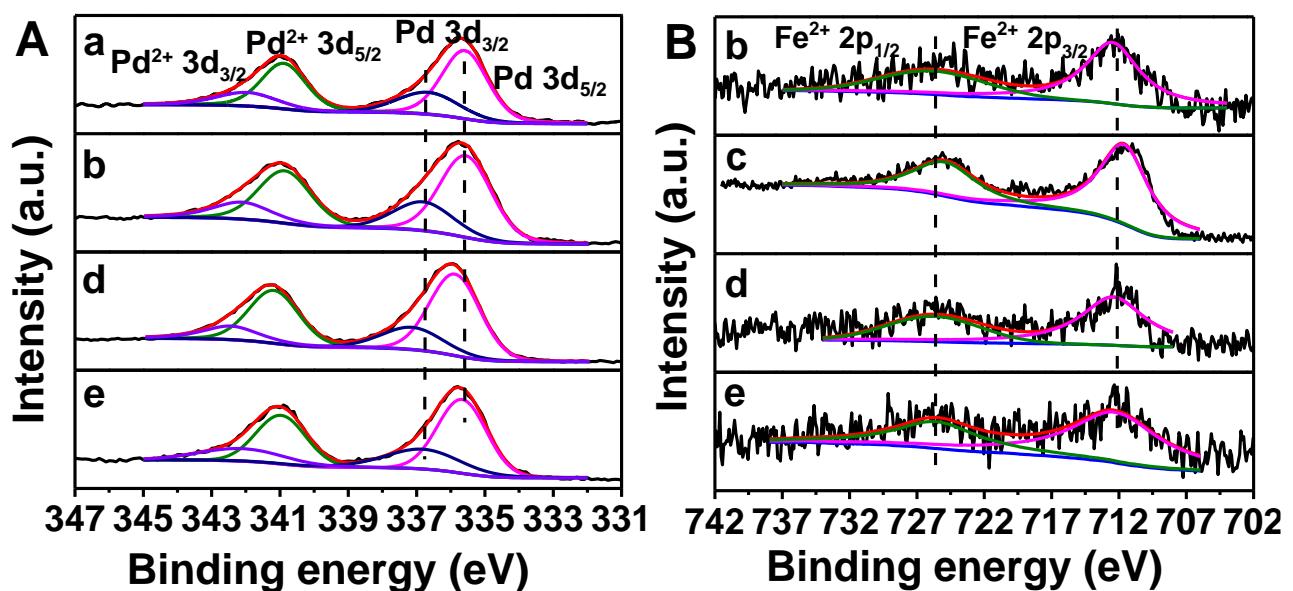


Figure S4. Pd 3d (A) and Fe 2p (B) spectra of the different catalysts a. $\text{Pd}_5/\text{Si-CODP}$, b. $\text{Pd}_5\text{Fe}_1/\text{Si-CODP}$, c. $\text{Fe}_1/\text{Si-CODP}$, d. $\text{Pd}_5/\text{Fe}_1/\text{Si-DP}$, e. $\text{Fe}_1/\text{Pd}_5/\text{Si-DP}$.

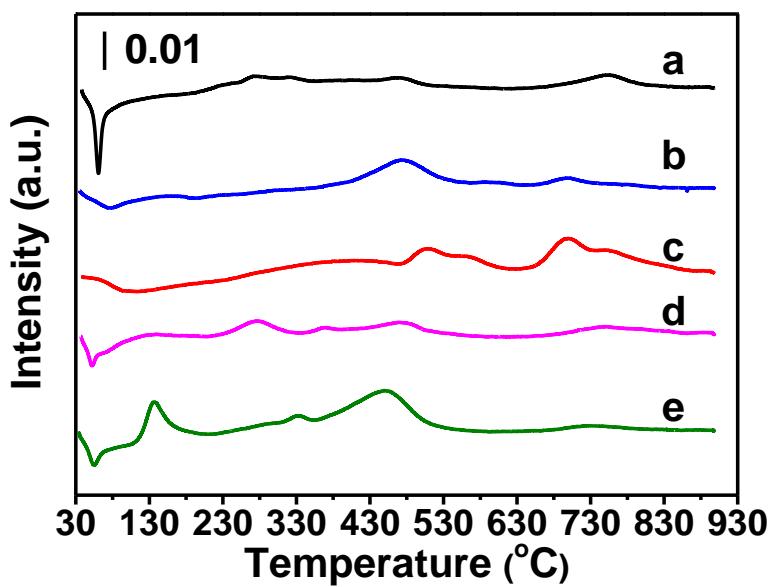
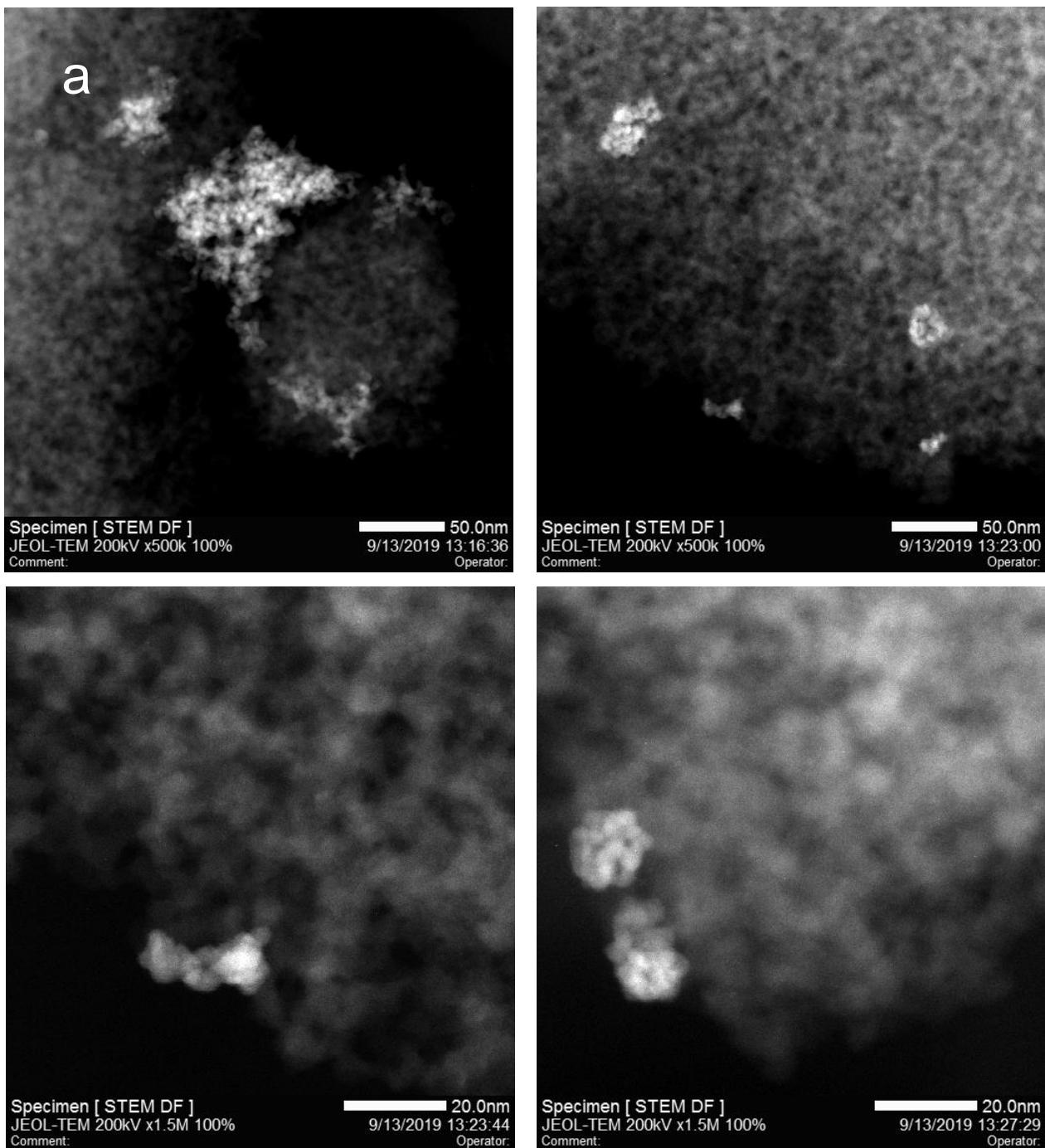
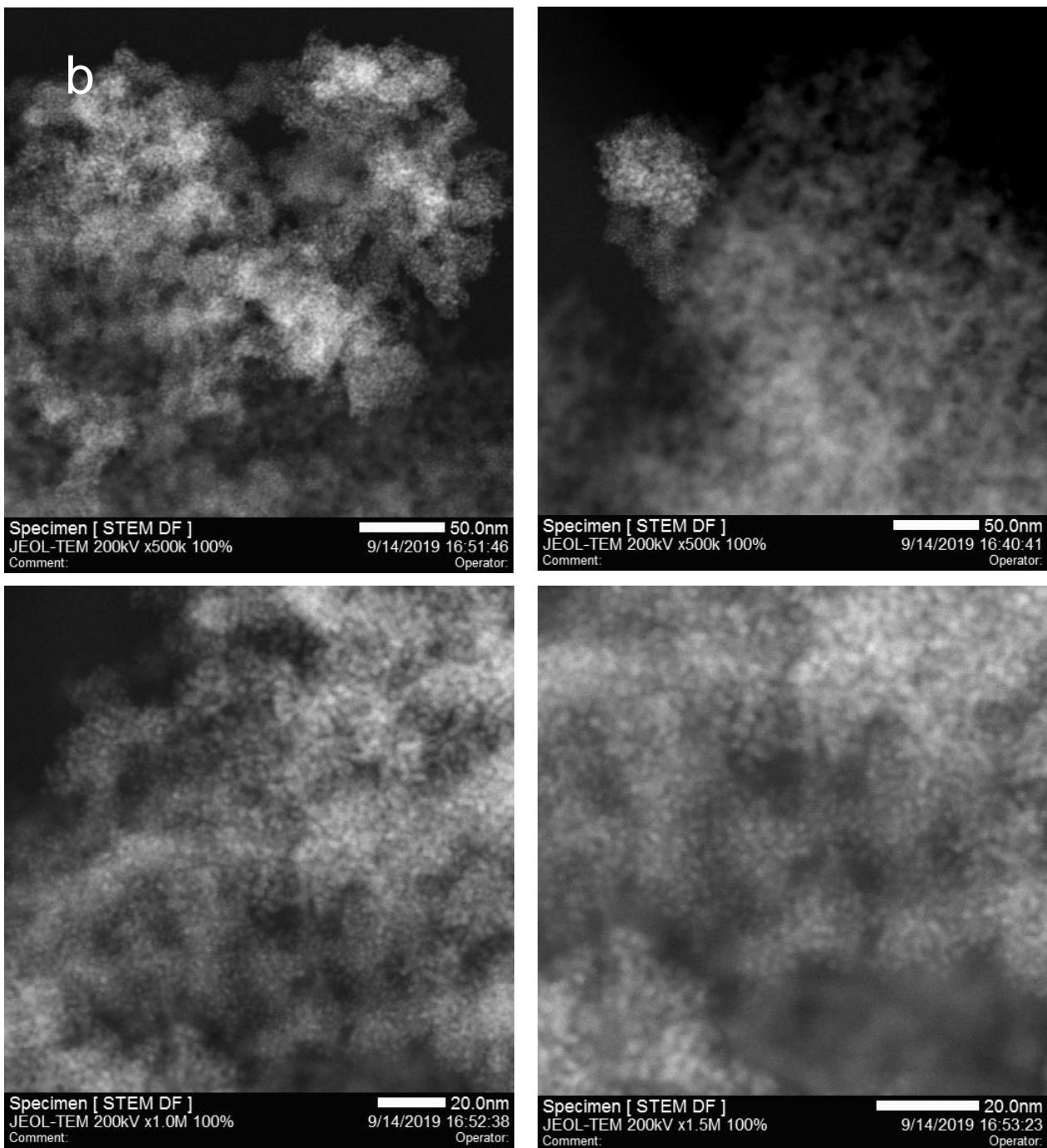
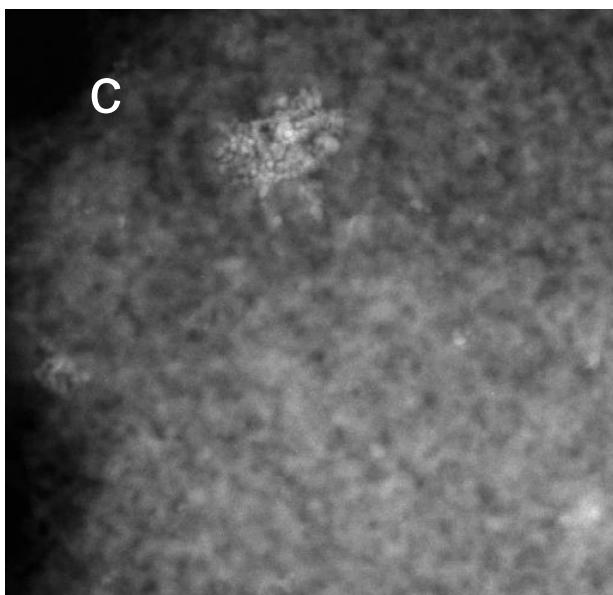


Figure S5. H₂-TPR curves of the catalysts a. Pd₅/Si-CODP, b. Pd₅Fe₁/Si-CODP, c. Fe₁/Si-CODP, d. Pd₅/Fe₁/Si-DP, e. Fe₁/Pd₅/Si-DP.

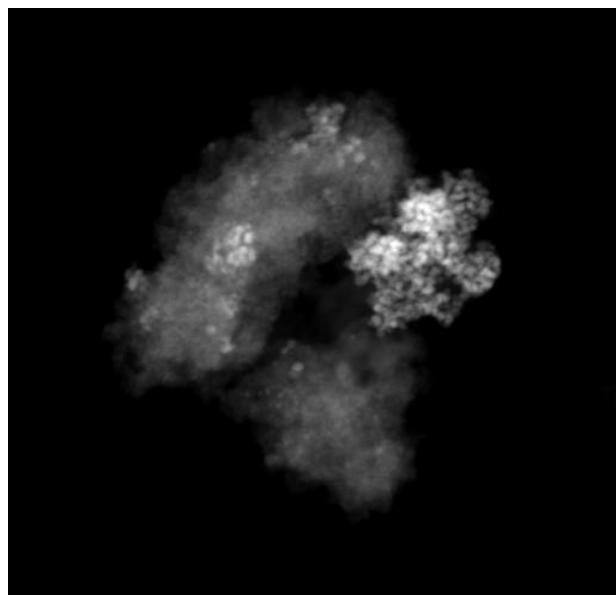






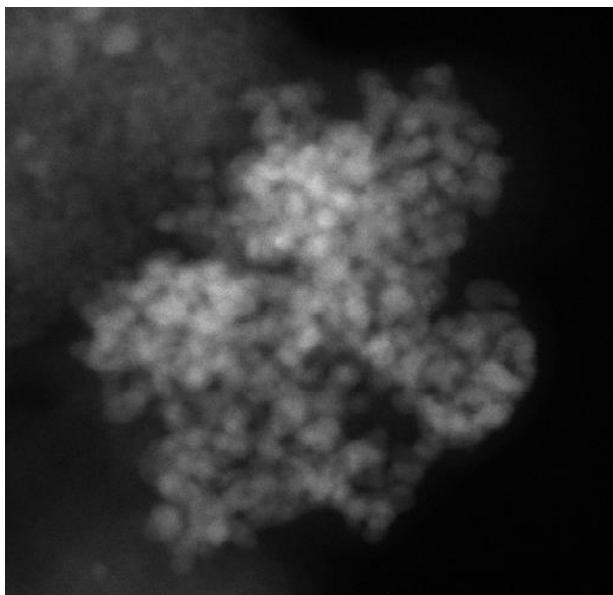
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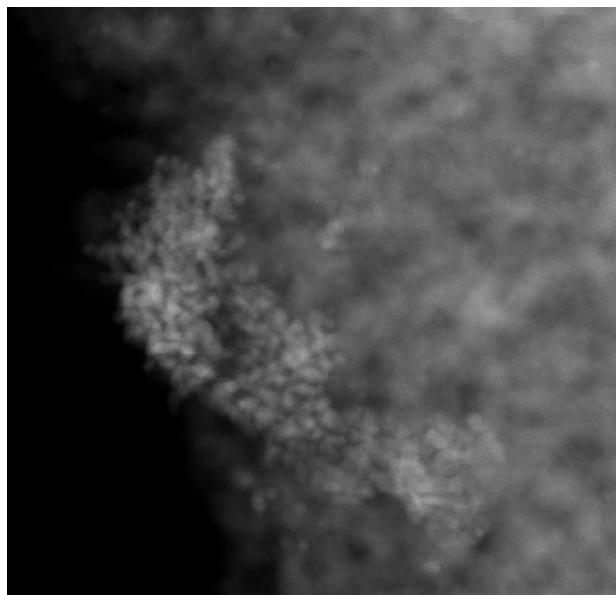
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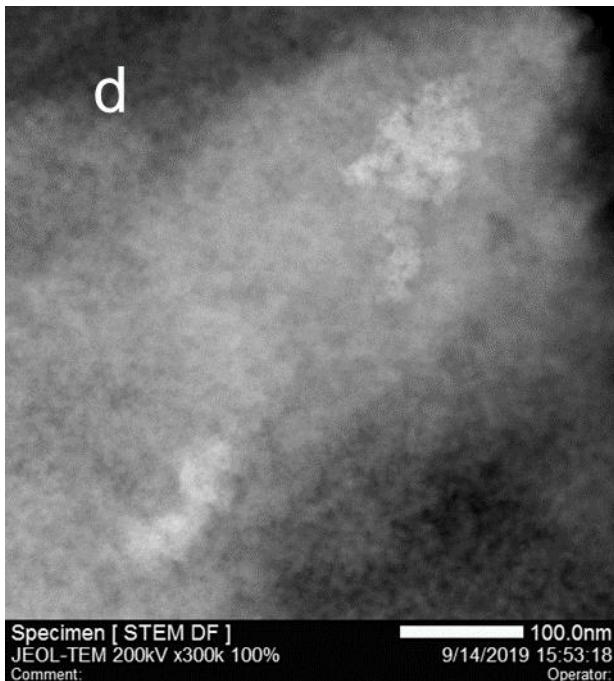
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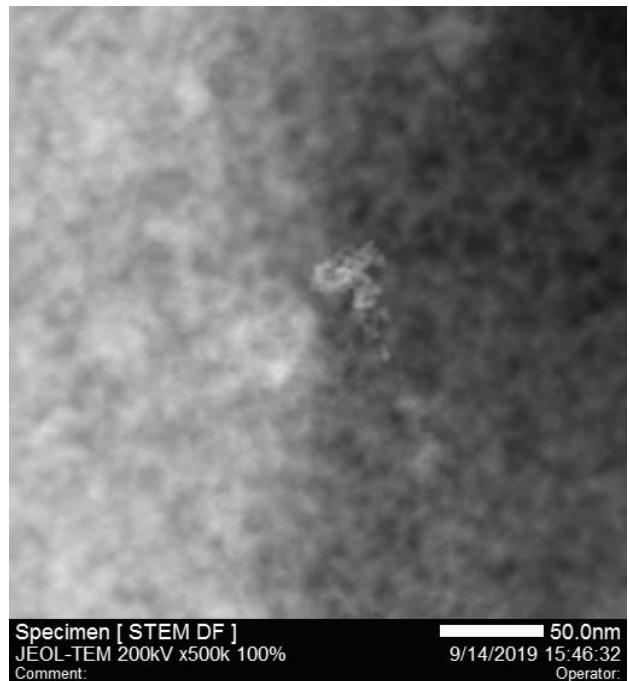
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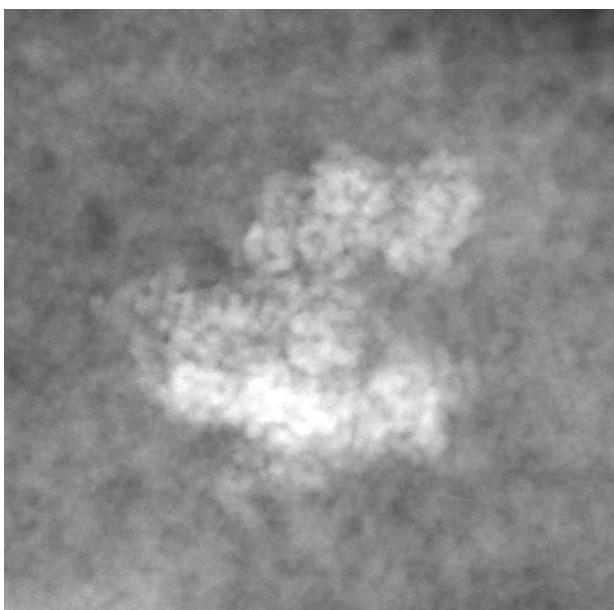
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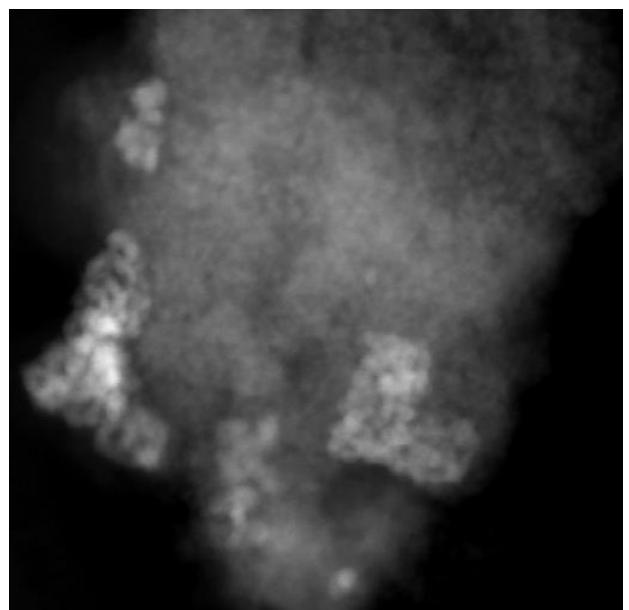
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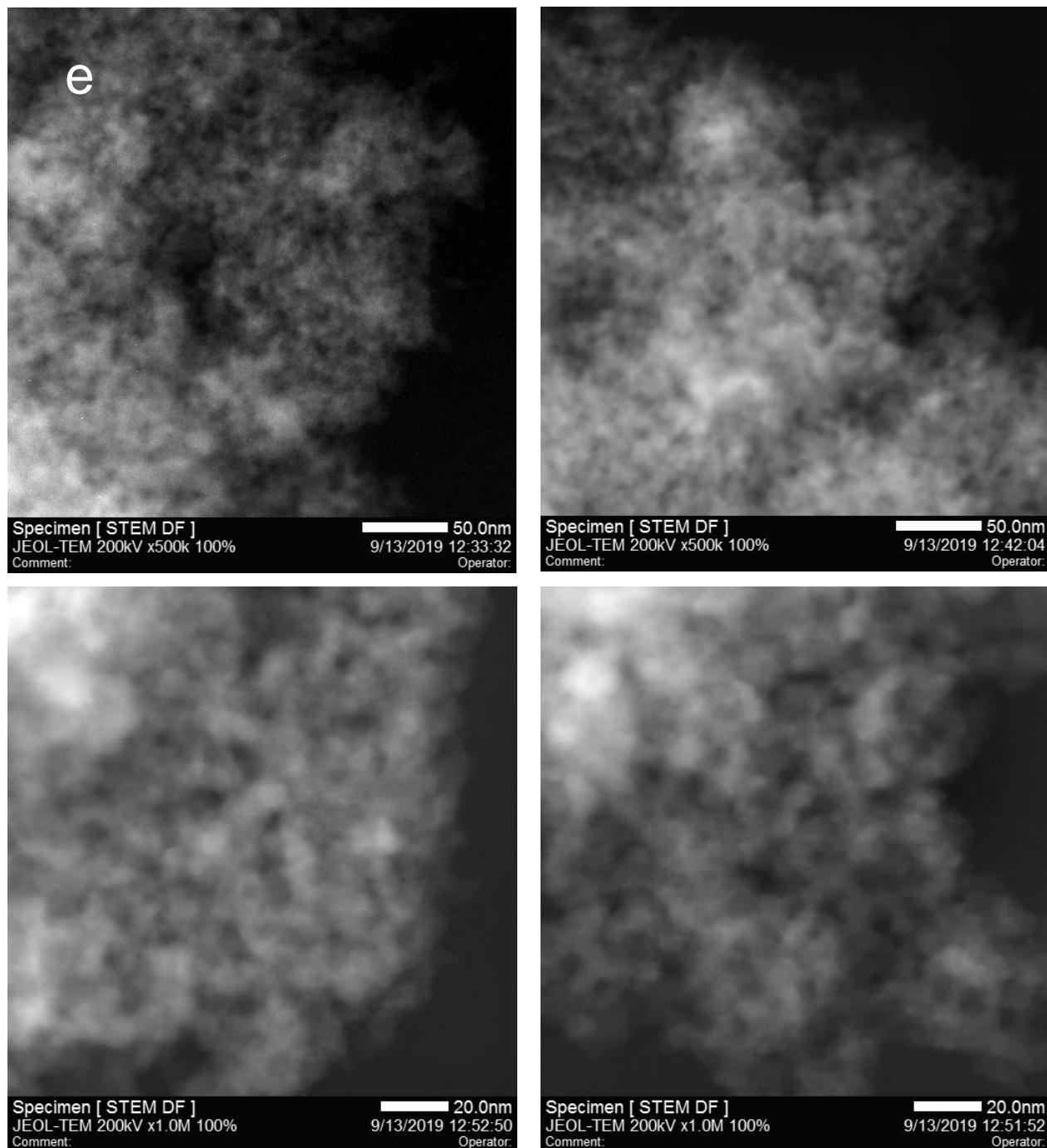


Figure S6. TEM images of the catalysts a. Pd₅/Si-CODP b. Pd₅Fe₁/Si-CODP, c. Pd₅/Fe₁/Si-DP, d. Fe₁/Pd₅/Si-DP, e. Fe₁/Si-CODP.

Fe₁/Pd₅/Si-DP, e. Fe₁/Si-CODP.

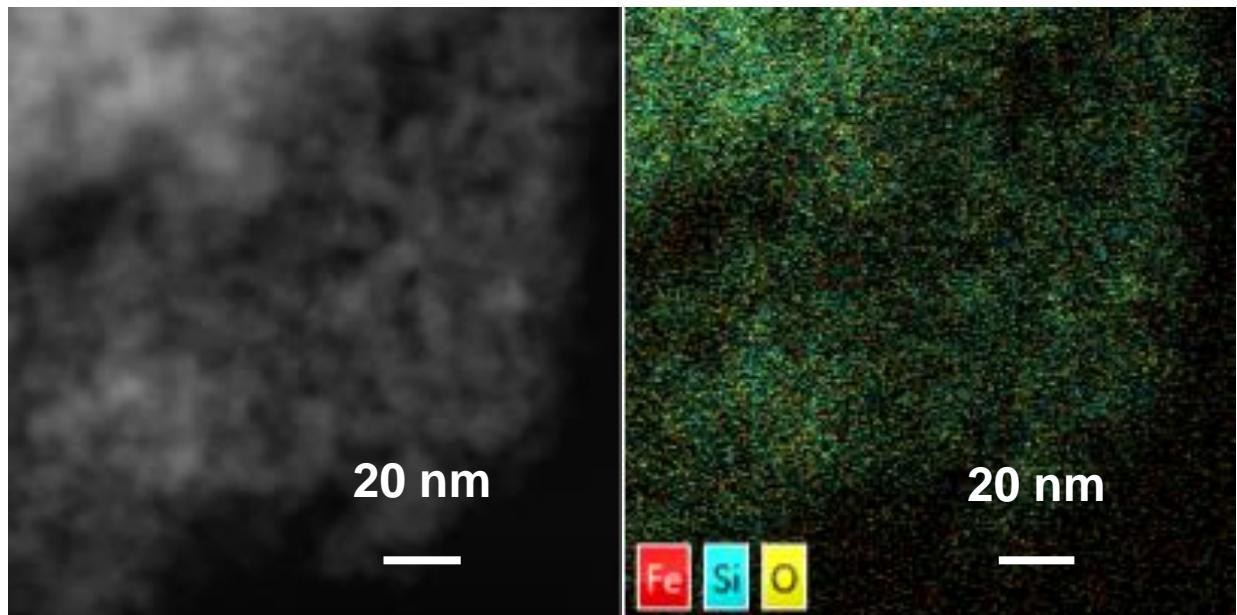


Figure S7. HAADF images and elemental mapping of Fe_1/Si -CODP.

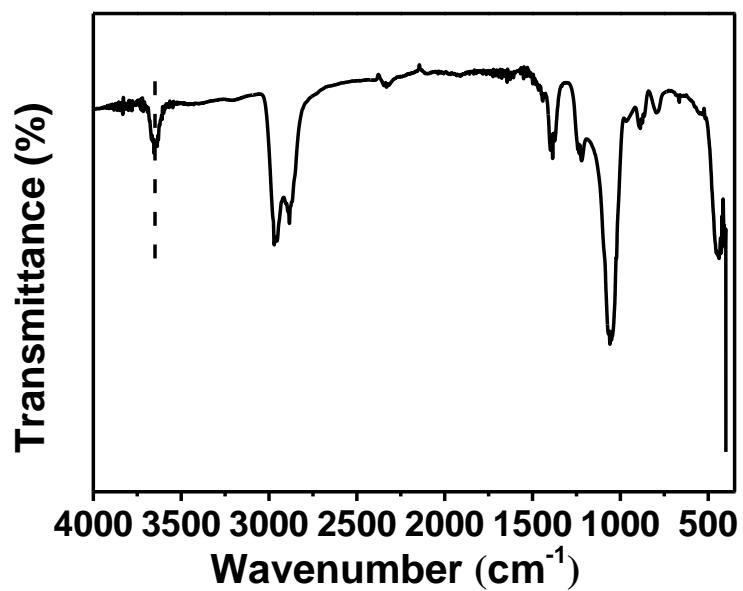


Figure S8. FTIR spectra of the support SiO_2 .

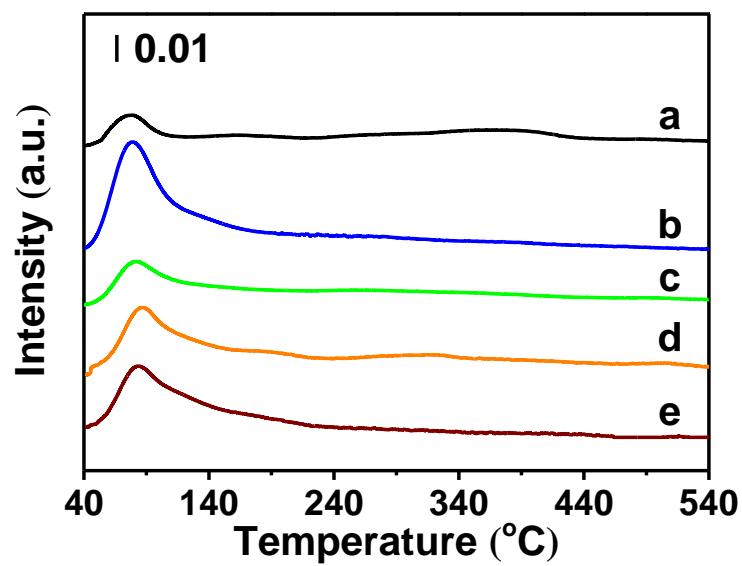


Figure S9. H₂-TPD profiles of the catalysts a. Pd₅/Si-CODP, b. Pd₅Fe₁/Si-CODP, c. Fe₁/Si-CODP, d. Pd₅/Fe₁/Si-DP, e. Fe₁/Pd₅/Si-DP.