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SUPPLEMENTARY INFORMATION

Direct generation of polypyrrole-coated palladium nanoparticles inside a metal-organic framework for semihydrogenation catalyst

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Supporting data



Figure S1. TEM images of (A) Pd(OAc)₂@MIL-101(12), (B) Pd(OAc)₂@MIL-101(24) and (C) Pd(OAc)₂@MIL-101(36).



Figure S2. (A) XRD patterns and (B) TG profiles of PdNPs/PPy@MIL-101.



Figure S3. UV-Vis diffuse reflectance spectra: (A) bulk PPy; (B) $Pd(OAc)_2@MIL-101(12)$ and PdNPs/PPy@MIL-101(12); (C) $Pd(OAc)_2@MIL-101(24)$ and PdNPs/PPy@MIL-101(24); (D) $Pd(OAc)_2@MIL-101(36)$ and PdNPs/PPy@MIL-101(36).



Figure S4. IR spectra of MIL-101, Pd(OAc)₂@MIL-101, PdNP/PPy@MIL-101 and bulk PPy.



Figure S5. (A) XRD pattern of PdNPs@MIL-101(24). (B) TG profile of PdNPs@MIL-101(24). (C) TEM image of PdNPs@MIL-101(24). (D) PdNP size distribution histogram of PdNPs@MIL-101(24).



Figure S6. (A) N_2 gas adsorption at 77 K and (B) pore size distribution of MIL-101, PdNPs/PPy@MIL-101(12), PdNPs/PPy@MIL-101(24) and PdNPs/PPy@MIL-101(36).

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Phenylacetylene conversion: 9%

Styrene selectivity: 100%

Figure S7. ¹HNMR chart of the reaction solution after 4 hours for the hydrogenation of phenylacetylene in the presence of PdNPs-PPy composite ([Pd] 0.05 mol%). The peaks corresponding to the alkene protons of styrene and the alkyne proton of phenylacetylene were marked with blue and orange circles, respectively.