

Supporting Information

One-step encapsulation of Pd nanoparticles in MOF via a temperature control program

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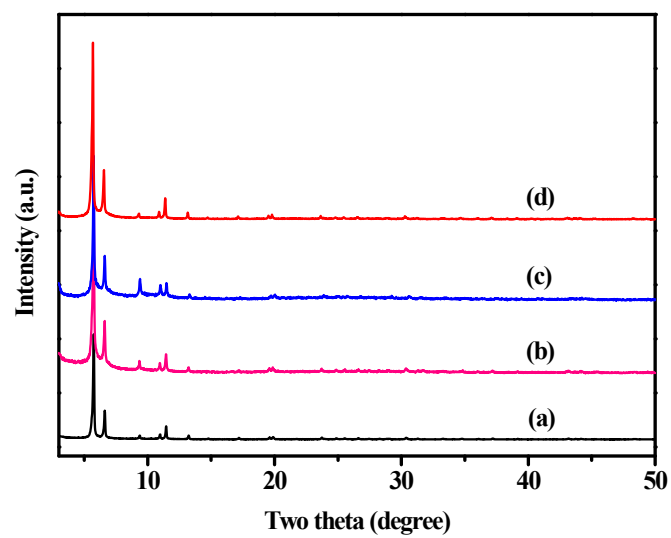


Figure S1. Powder XRD patterns of UiO-67 samples: (a) UiO-67, (b) Pd^{II}-in-UiO-67, (c) Pd-in-UiO-67, and (d) Pd-in-UiO-67 after reaction.

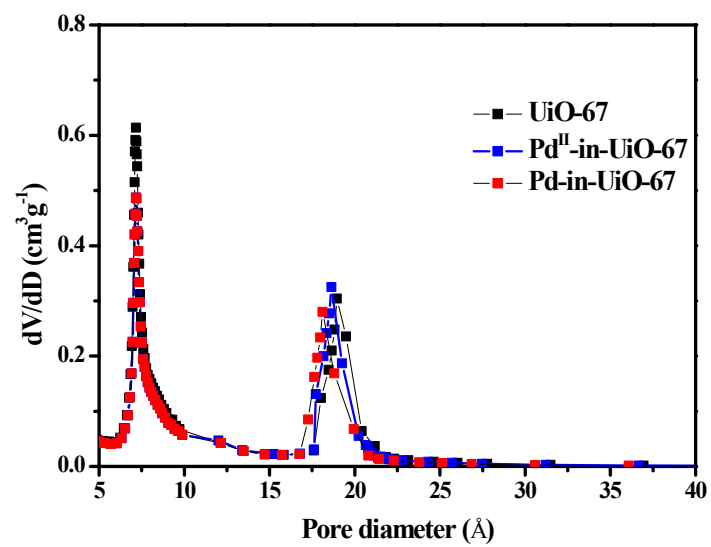


Figure S2. Pore-size distribution curves of the as-synthesized UiO-67, Pd^{II}-in-UiO-67, and Pd-in-UiO-67.

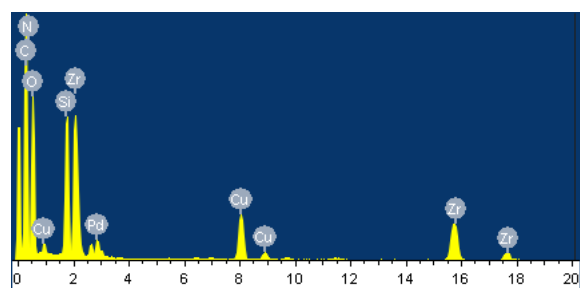


Figure S3. The EDX pattern of Pd-in-UiO-67.

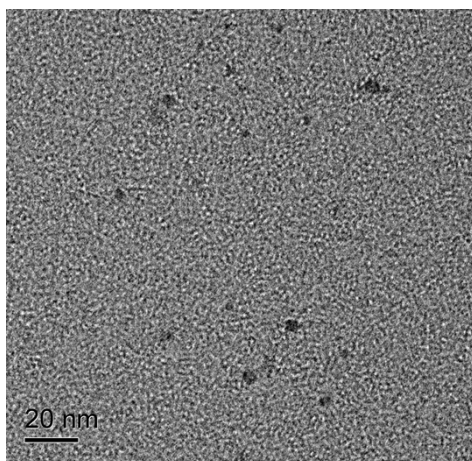


Figure S4. TEM image of unsupported Pd NPs prepared in DMF at 130 °C.

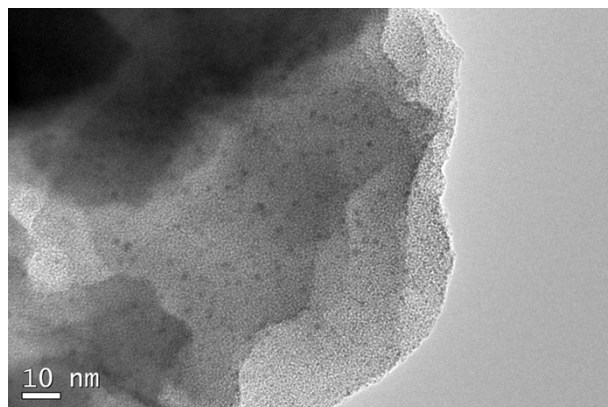


Figure S5. TEM image of Pd-in-UiO-67 synthesized by heating at 80 °C for 20 hours and 130 °C for 20 hours.

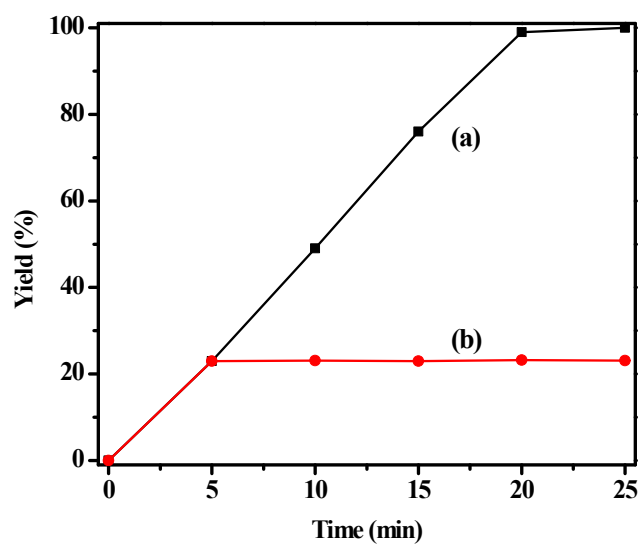


Figure S6. Activity profile for the reduction of styrene to ethylbenzene. Reaction conditions: styrene (0.1 mmol), Pd-in-UiO-67 (1% Pd), THF (2 mL), 1 atm H₂, 25 °C. (a) With catalyst, and (b) with filtrate.

Table S1. Surface areas and pore volumes of the MOF samples.

Sample	S_{BET} ($\text{m}^2 \text{ g}^{-1}$)	S_{Langmuir} ($\text{m}^2 \text{ g}^{-1}$)	V_{pore} ($\text{cm}^3 \text{ g}^{-1}$)
UiO-67	2408	3045	1.09
Pd ^{II} -in-UiO-67	2008	2577	0.91
Pd-in-UiO-67	2163	2766	0.99

Table S2. Results of hydrogenation of styrene.^a

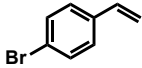
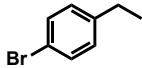
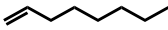
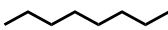
Entry	Catalyst	Time (min)	Yield (%)
1	1% Pd-in-UiO-67	25	100
2	2% Pd-in-UiO-67	20	100
3	3% Pd-in-UiO-67	15	100
4	4% Pd-in-UiO-67	20	100

^a Reaction conditions: styrene (0.1 mmol), catalyst (Pd 1 mol%), THF (2 mL), 1 atm H₂, 25 °C.

Table S3. Comparison of Pd-in-UiO-67 with other catalysts in the hydrogenation of styrene.

Catalyst	T (°C)	P_{H_2} (atm)	Time (min)	Yield (%)	Ref.
Pd-in-UiO-67	25	1	15	100	This work
Pd/Tm-MOF	35	1	720	>99	1
Pd/BTP-POF	25	1	120	100	2
Pt/15TS	60	40	60	100	3
Pd/PEG	25	1	90	100	4
Pd(OAc) ₂ @MONT	25	1	60	>99	5
Pd@PPI/SiO ₂	70	30	15	100	6
Pd@MOF	30	1	1800	100	7
Pd@CPP-F1	40	1.5	240	100	8
Pd/Fe ₂ O ₃	25	1	120	83	9
Pd-Pt/CNT	25	1	30	99	10

Table S4. Hydrogenation of various olefins catalyzed by 1.0% Pd-in-UiO-67.^a

Entry	Substrate	Product	Time (min)	Yield (%) ^b
1			20	100
2			15	100
3			15	100
4			20	100

^a Reaction conditions: styrene (0.1 mmol), catalyst (Pd 1 mol%), THF (2 mL), 1 atm H₂, 25 °C. ^b The yield was determined by GC-MS analysis.

References

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