Supporting Information

Ultrafine PdCo bimetallic nanoclusters confined in N-doped porous carbon for the efficient semi-hydrogenation of alkynes

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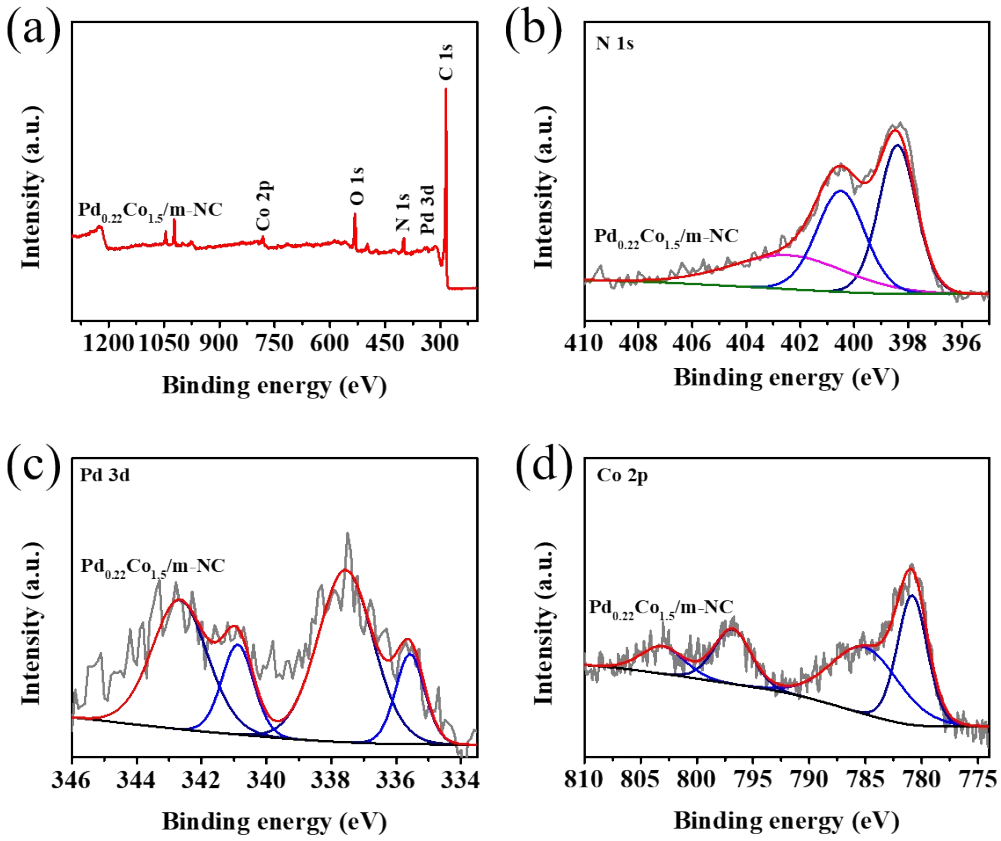

Figure S1. (a) The full-range XPS spectrum of $Pd_{0.22}Co_{1.5}$/m-NC. The XPS spectra of N 1s (b), Pd 3d (c) and Co 2p (d) of $Pd_{0.22}Co_{1.5}$/m-NC.

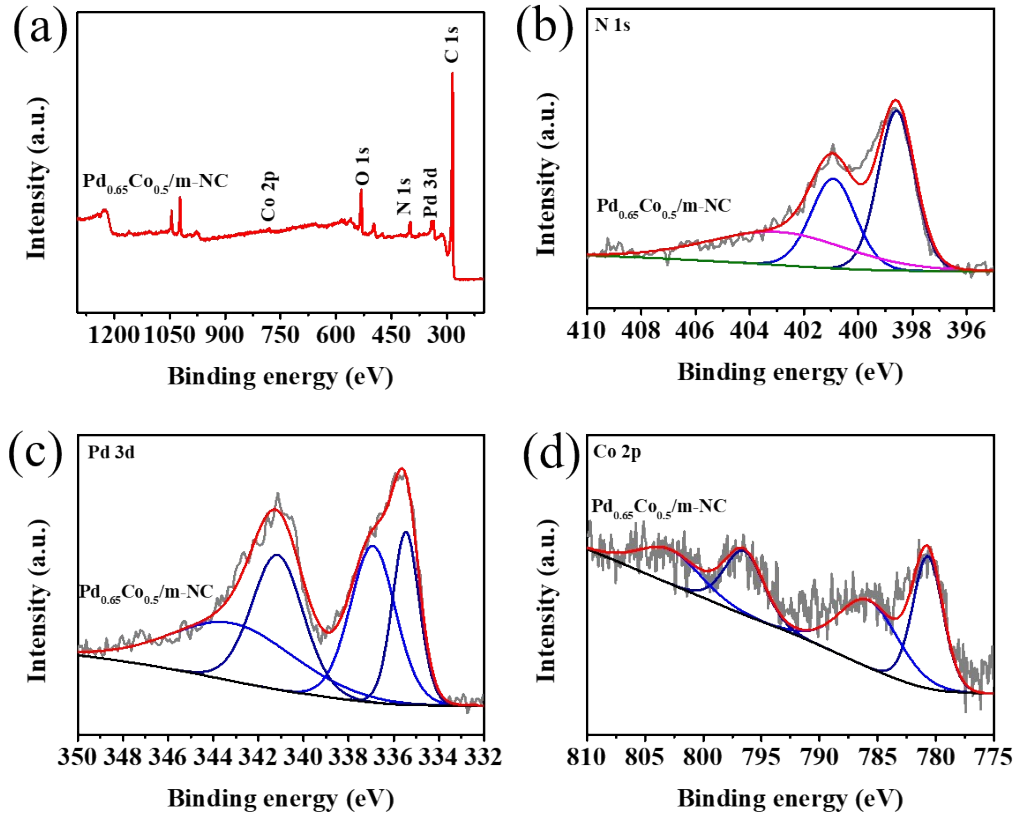

Figure S2. (a) The full-range XPS spectrum of $Pd_{0.65}Co_{0.5}$/m-NC. The XPS spectra of N 1s (b), Pd 3d (c) and Co 2p (d) of $Pd_{0.65}Co_{0.5}$/m-NC.

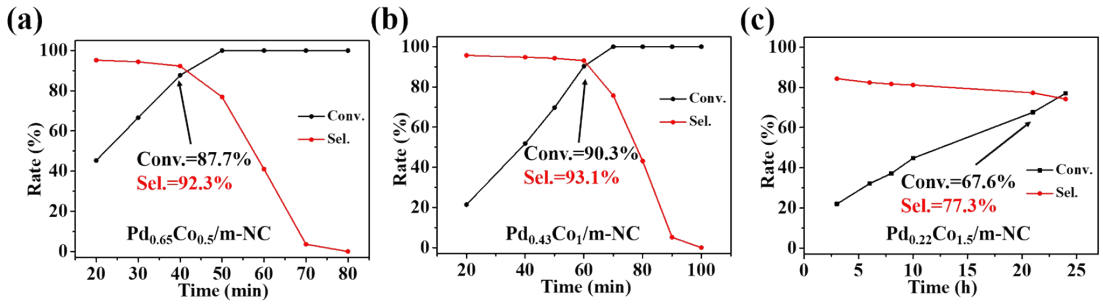

Figure S3. The trend of conversion and selectivity of phenylacetylene semi-hydrogenation reaction catalyzed by (a) $Pd_{0.65}Co_{0.5}$/m-NC, (b) $Pd_{0.43}Co_1$/m-NC and (c) $Pd_{0.22}Co_{1.5}$/m-NC under same conditions (10 mg catalyst, 1 mmol phenylacetylene, 5 mL ethanol, room temperature, 1 atm H_2).

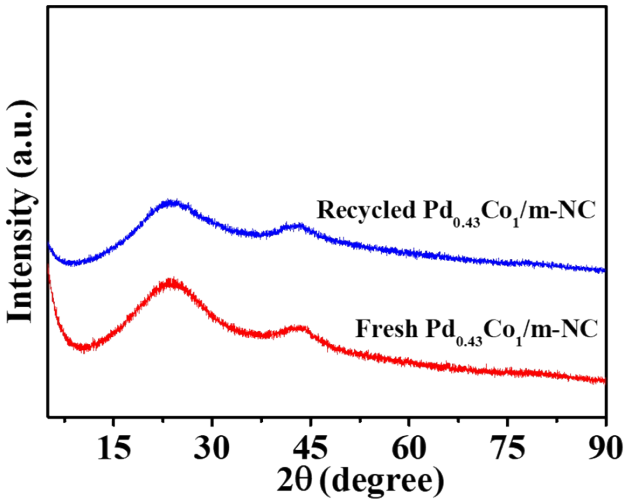

Figure S4. PXRD pattern of fresh $Pd_{0.43}Co_1$/m-NC and recycled $Pd_{0.43}Co_1$/m-NC.

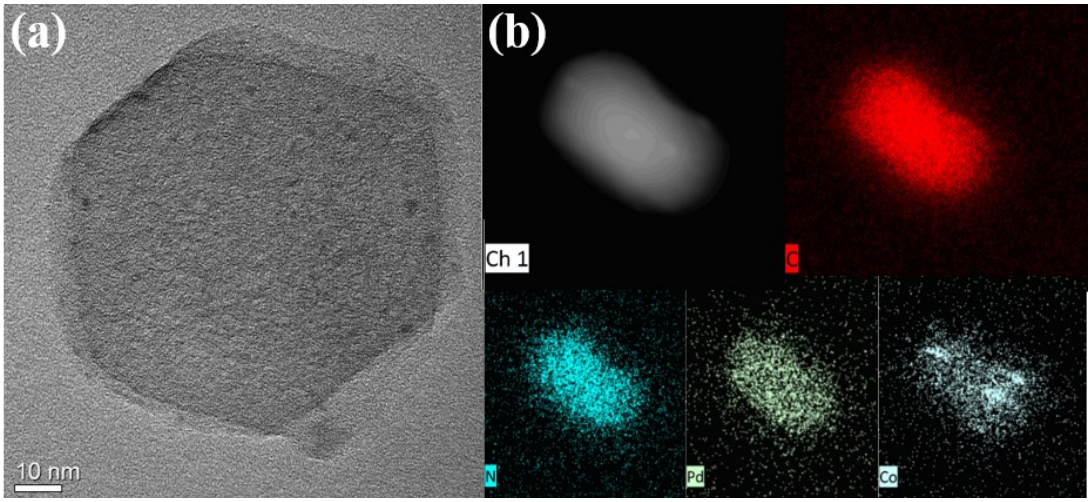

Figure S5. (a) TEM images of the recycled $Pd_{0.43}Co_1$/m-NC and histogram of the distribution of PdCo NCs. (b) EDX mapping of composition element C, N, Pd and Co in recycled $Pd_{0.43}Co_1$/m-NC.

Table S1. BET surface area and pore structure characterization parameters of materials.

Samples	BET surface area ($m^2 \cdot g^{-1}$)	t-Plot micropore area ($m^2 \cdot g^{-1}$)	Pore volume ($cm^3 \cdot g^{-1}$)	t-Plot micropore volume ($cm^3 \cdot g^{-1}$)	Average pore size (nm)
m-NC	1008.93	637.7	0.39	0.32	2.51
$Pd_{0.43}Co_1$/m-NC	1132.41	727.5	0.49	0.36	2.65

Table S2. Fitting data for H_2-TPD spectra of different materials.

Samples	Peak type	Center Grvty	Area Intg	FWHM
Co_1/m-NC	Gaussian	432.2	2.6	126.7
	Gaussian	681.9	1.4	55.8
$Pd_{0.43}$/m-NC	Gaussian	484.1	11.2	177.5
$Pd_{0.43}Co_1$/m-NC	Gaussian	492.7	19.1	196.4

Table S3. Comparison the catalytic performance for semi-hydrogenation of alkynes presented in literatures and this work.

Entry	Catalyst	Substrate	T (℃)	P (MPa)	Conv. (%)	Alkene Sel. (%)	Ref.
1	Pd/C	2-Butyne-1,4-diol	65	0.3	65	73	[1]
2	PdCu/ZnO	Dehydroisophytol	80	0.4	99	95-97	[2]
3	PdAg/ZnO	Dehydroisophytol	80	0.4	99	97-98	
4	UiO-67@Pd@UiO-67 (50 nm)	phenylacetylene	10	0.5	＞99	93.1	[3]
5	Pd/Al_2O_3	acetylene	200	-	43	17	[4]
6	PdGa	acetylene	200	-	86	75	
7	PdZn/CN@ZnO	Dehydroisophytol	50	1.0	96	＞99	[5]
8	$PdZn/Al_2O_3$	2-Methyl-3-butyn-2-ol	100	0.1	25	90	[6]
9	Pd-Ru@ZIF-8	phenylacetylene	100	0.1	98	96	[7]
10	$PdIn/MgAl_2O_4$	phenylacetylene	25	0.1	92	97	[8]
11	This work	phenylacetylene	R.T.	0.1	＞99	93.6	-

Reference

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