Supplementary Information

Confined thermal transformation strategy to synthesize single atom catalysts supported on nitrogen-doped mesoporous carbon nanospheres for selective hydrogenation

Zhengbin Tian,[a,b] Wenquan Wang,[a,b] Yan Zheng[a] and Guang-Hui Wang*[a,b]

[a] Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, 266101 Qingdao, China.

[b] University of Chinese Academy of Sciences, 100049 Beijing, China

*E-mail: wanggh@qibebt.ac.cn

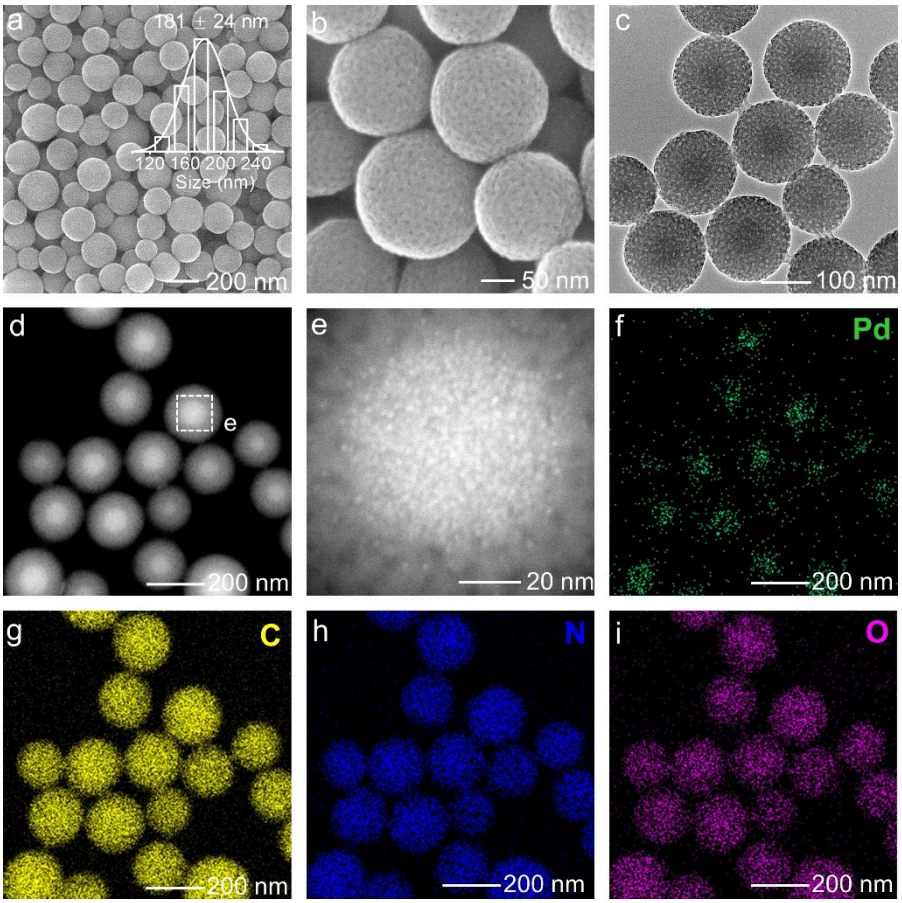

Fig. S1 (a,b) SEM images, (c) TEM image, (d-i) HAADF-STEM and the corresponding EDS elemental mapping images of Pd-NCs@NMPS-0.

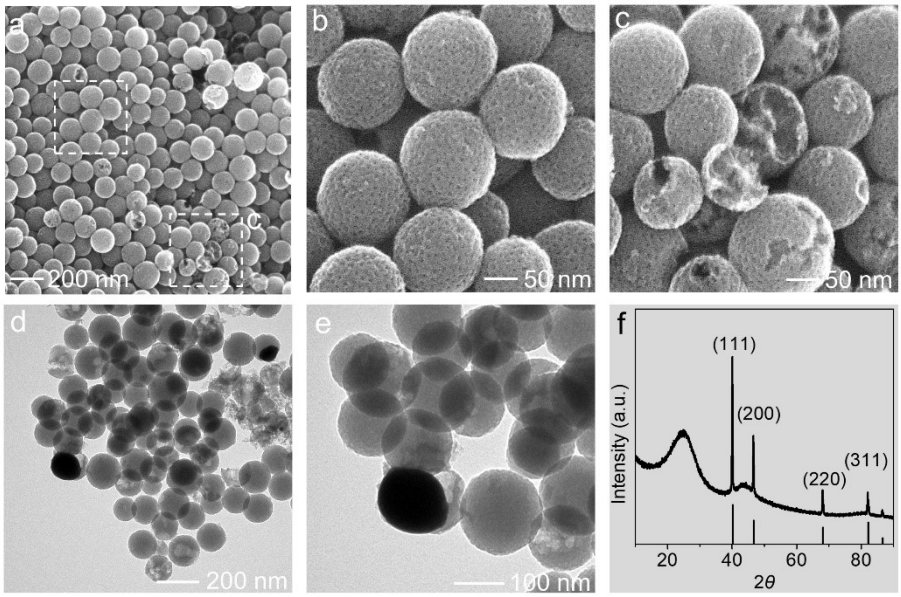

Fig. S2 (a-c) SEM images, (d,e) TEM images and (f) XRD pattern of Pd-NCs@NMPS-0 after pyrolysis at 800 °C under a NH_3/Ar (5%/95%) flow.

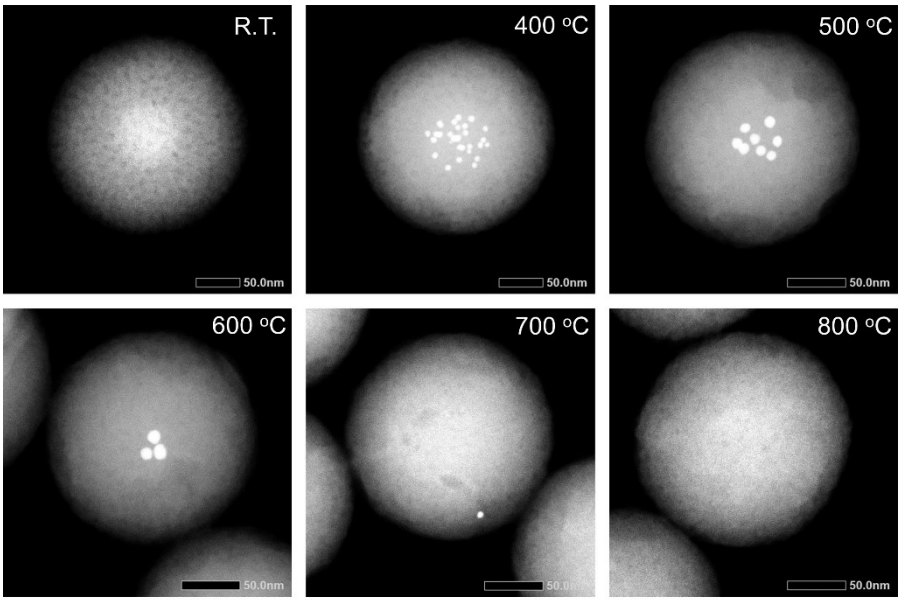

Fig. S3 Ex situ HAADF-STEM images of Pd-NCs@NMPS after pyrolysis at different temperature.

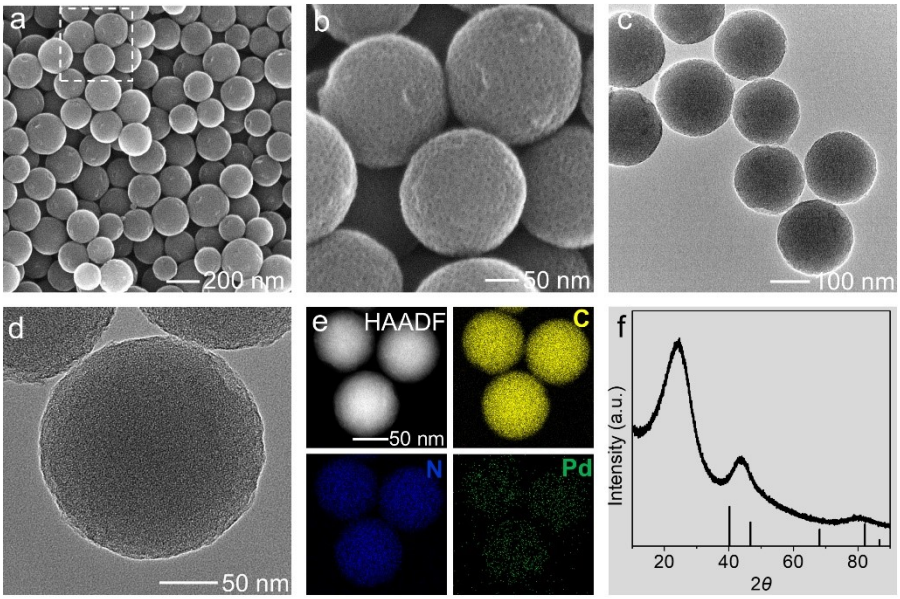

Fig. S4 (a,b) SEM images, (c,d) TEM images, (e) HAADF-STEM and the corresponding EDS elemental mapping images, (f) XRD pattern of Pd_1/NMCS-Ar.

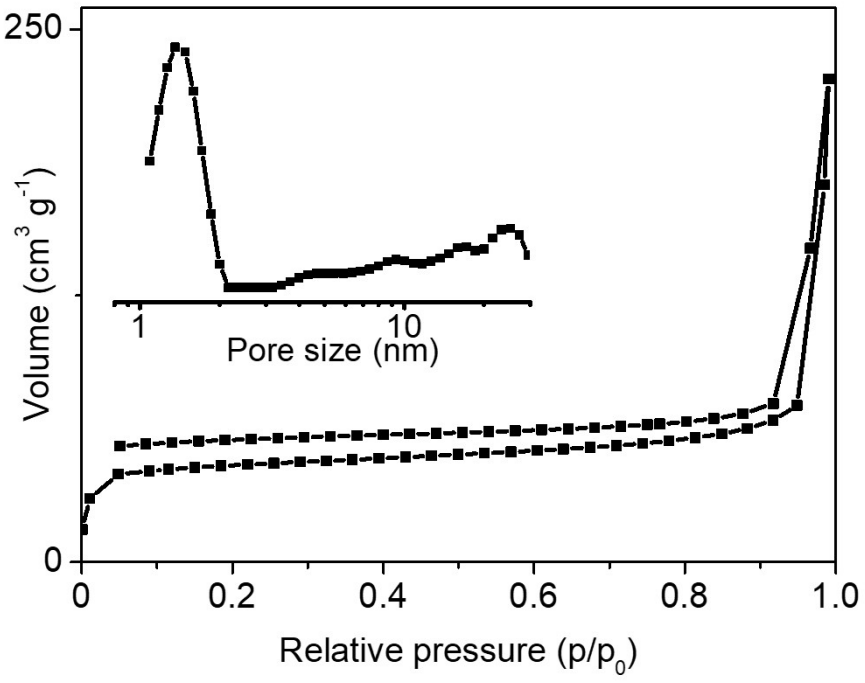

Fig. S5 N_2-sorption isotherm and the pore size distribution of Pd_1/NMCS-Ar.

It is found that the adsorption and desorption branches are not closed for the sample of Pd_1/NMCS-Ar. The phenomenon is often observed for the samples of porous polymers and nitrogen-doped carbons (*Angew. Chem. Int. Ed.* **2016**, *55*, 8850-8855).

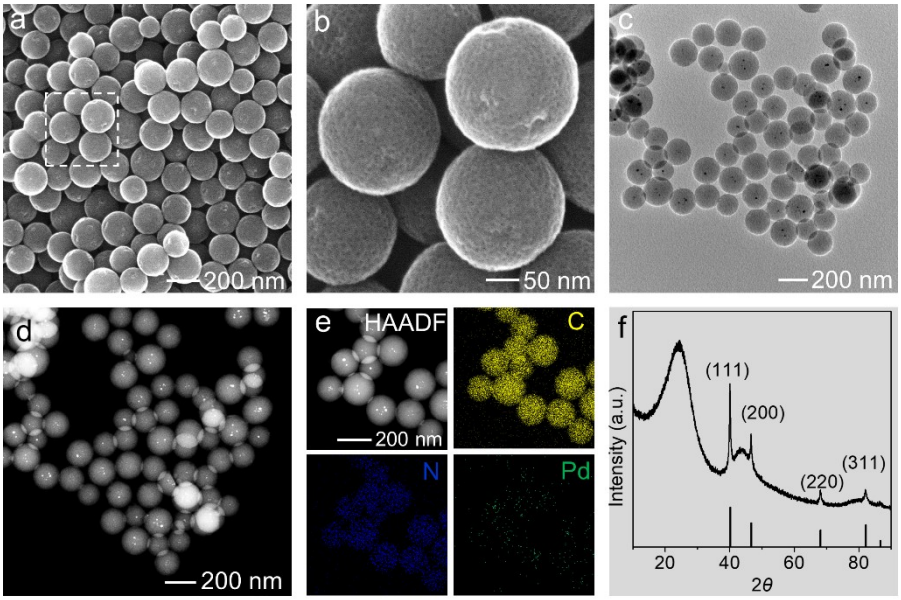

Fig. S6 (a,b) SEM images, (c) TEM image, (d,e) HAADF-STEM and the corresponding EDS elemental mapping images, (f) XRD pattern of Pd@NMCS-H_2.

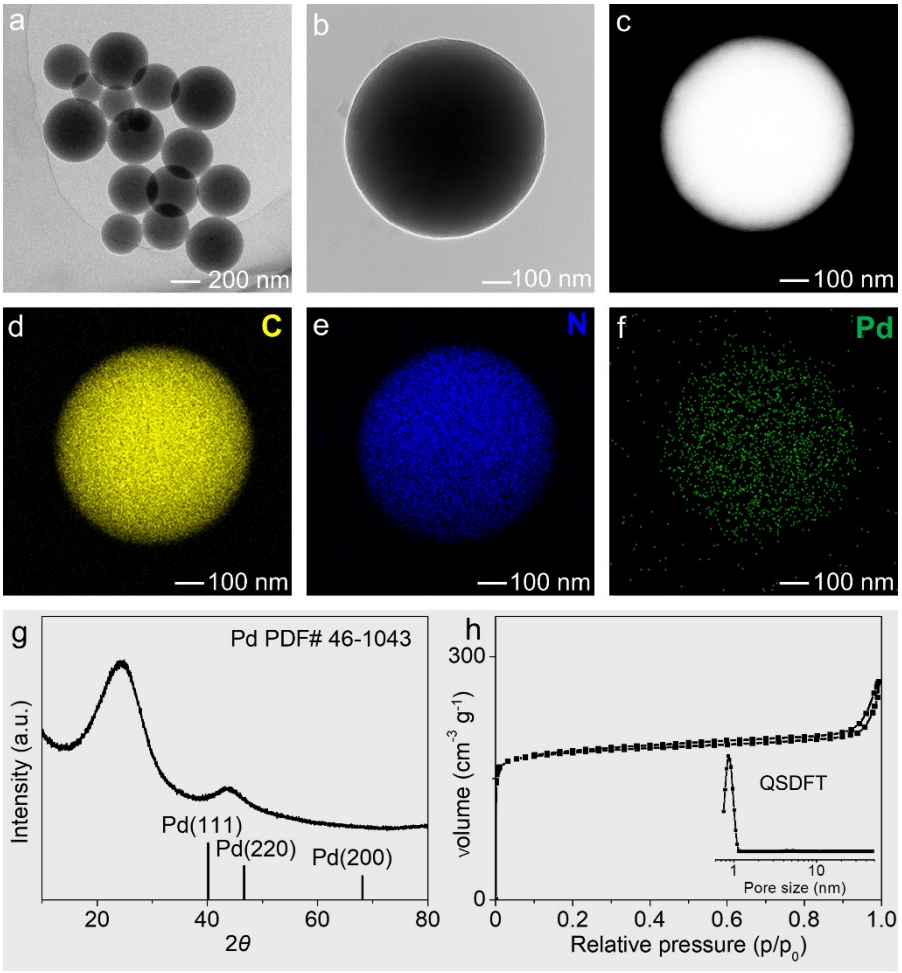

Fig. S7 (a,b) TEM images, (c-f) HAADF-STEM and the corresponding EDS elemental mapping images, (g) XRD pattern and (h) N_2-sorption isotherm and the pore size distribution (inset) of Pd_1/NCS.

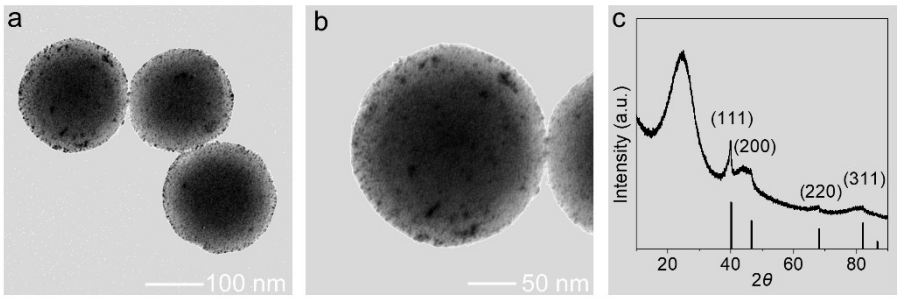

Fig. S8 (a,b) TEM images and (c) XRD pattern of Pd-NPs/NMCS.

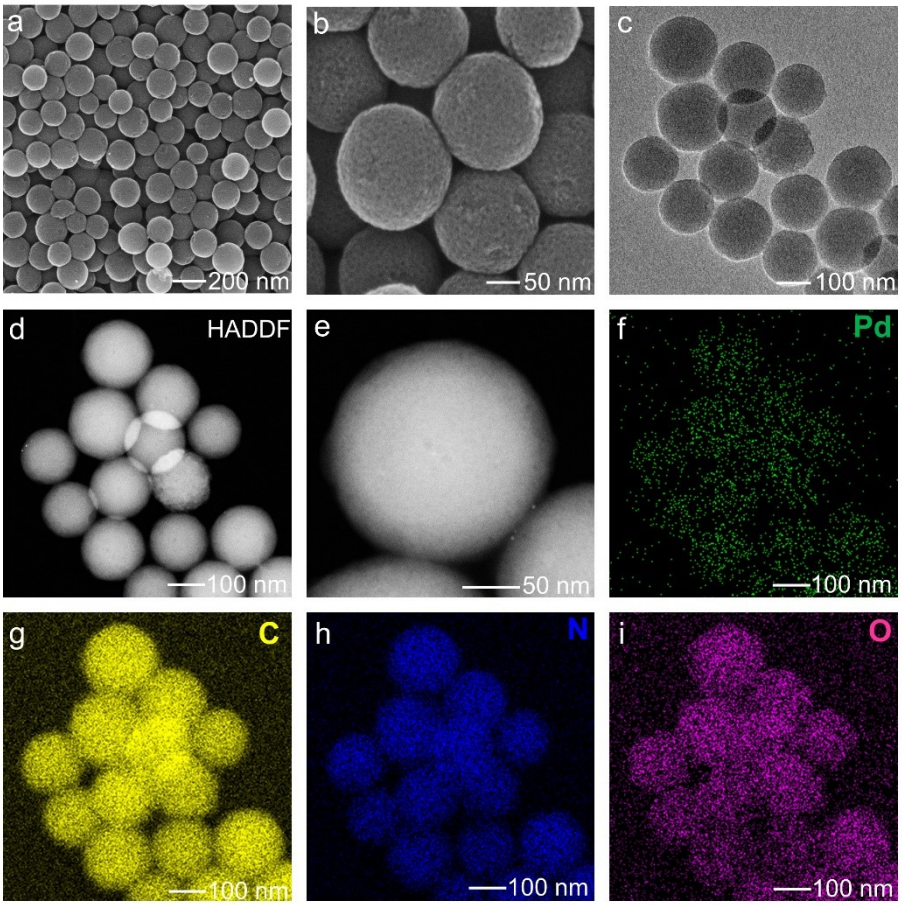

Fig. S9 (a,b) SEM images, (c) TEM image, (d-i) HAADF-STEM and the corresponding EDS elemental mapping images of Pd_1/NMCS after five runs.

Table S1. Textural parameters of the nitrogen-doped carbon catalysts.

Sample	Nanospheres size (nm)	Textual properties		Chemical composition			
		S_{BET} (m^2 g^{-1})	V_{total} (cm^3 g^{-1})	N [a] wt%	C [b] wt%	N [b] wt%	O [b] wt%
Pd_1/NMCS	~177	595	0.46	9.3	84.2	10.2	3.5
Pd_1/NMCS-Ar	~193	167	0.32	6.5	85.6	8.8	4.0
Pd@NMCS-H_2	~178	482	0.57	4.2	86.0	6.1	6.8
Pt_1/NMCS	~144	590	0.54	9.1	--	--	--
Pd_1/NCS	100~1000	728	0.42	8.9	--	--	--

[a] Measured by elemental analysis; [b] Measured by XPS.