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Electronic Supplementary Information

Creating Extra Pores in Microporous Carbon via a Template Strategy for Remarkable Enhancement of Ambient-Pressure CO_2 Uptake

Baiyan Li,[a] Yiming Zhang,[a,b,*] Dingxuan Ma,[b] Liangkui Zhu,[b] Daliang Zhang,[b] Matthew Chrzanowski,[a] Zhan Shi[b] and Shengqian Ma[a,*]

[a]Department of Chemistry, University of South Florida, 4202 East Fowler Avenue, Tampa, Florida, 33620, United States, Fax: +1 813-974-3203; Tel: +1 813-974-5217;

[b]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, People's Republic of China

E-mail: sqma@usf.edu; zhangyiming0805@gmail.com

1. Experimental Details

All reagents were purchased from Sigma-Aldrich or Alfa and used as received unless otherwise indicated. Tetrakis(4-bromophenyl)silane[1] and PPN-4[2] were synthesized according to the procedures reported in literature.

1.1 Synthesis of PPN-4

To a solution of 2,2'-bipyridyl (1.41 g, 9.04 mmol), bis(1,5-cyclooctadiene)nickel(0) ($Ni(COD)_2$, 2.5 g, 9.04 mmol), and 1,5-cyclooctadiene (COD, 0.18 mL, 9.12 mmol) in anhydrous DMF/THF (150 mL/225 mL) add tetrakis(4-bromophenyl)silane (1.27 g, 2.0 mmol), and the mixture was stirred at room temperature under argon atmosphere overnight. Then, the mixture was cooled in ice bath, 6 mol/L HCl solution (125 mL) was added, the resulting mixture was stirred for another 12 h. the precipitate was collected, then washed with Methanol (6 × 100 mL), and H_2O (6 × 100 mL), respectively, and dried in vacuo to produce PPN-4 as off-white powder.

1.2 Synthesis of PPN-4/C600

The powder of PPN-4 was heat-treated in a horizontal quartz reactor under an N_2 flow, and heated to 600 ºC with a heating rate of 5 ºC/min, the sample was pyrolyzed at 600 ºC for 8 h to afford the carbon material designated as PPN-4/C600-Si. Then the obtained PPN-4/C600-Si was soaked into a 2 M KOH solution at 120 ºC under hydrothermal conditions for two days followed by washing with water and methanol to afford the final microporous carbon material designated as PPN-4/C600.

1.3 Synthesis of PPN-4/C800 and PPN-4/C1000

The synthesis procedures of PPN-4/C800 and PPN-4/C1000 were similar to PPN-4/C600 except the heat-treated temperature at 800 ºC and 1000 ºC respectively.

2. Characterizations

PXRD patterns were collected on a Bruker D8 Advance X-ray diffractometer. Gas sorption experiments were carried out on a surface area analyzer ASAP-2020. N_2 gas

sorption isotherms were measured at 77 K using a liquid N_2 bath. CO_2 sorption isotherms were collected at 273 K using a water-ice bath and at 295 K with a water bath. Prior to the measurements, the samples were degassed for 10 h at 180 °C.

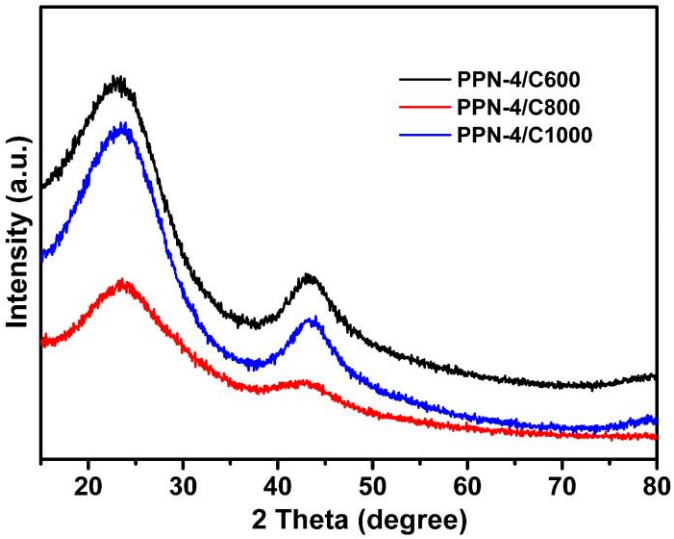

Fig. S1. Powder XRD patterns of the porous carbons PPN-4/C600, PPN-4/C800 and PPN-4/C1000.

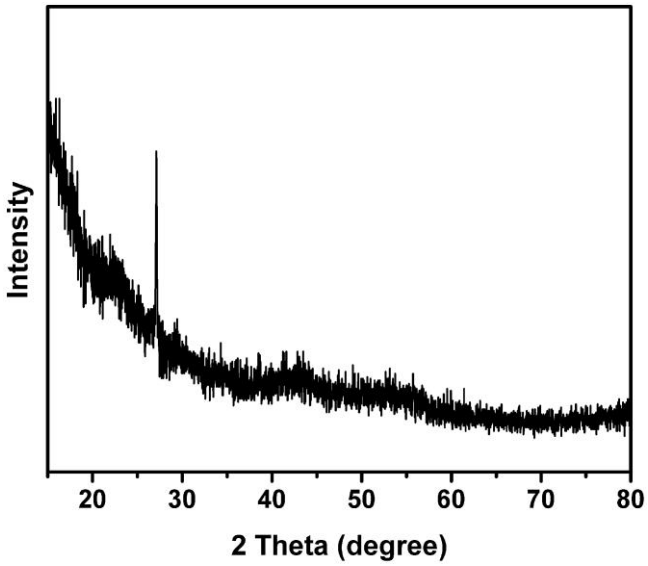

Fig. S2. Powder XRD patterns of the PPN-4.

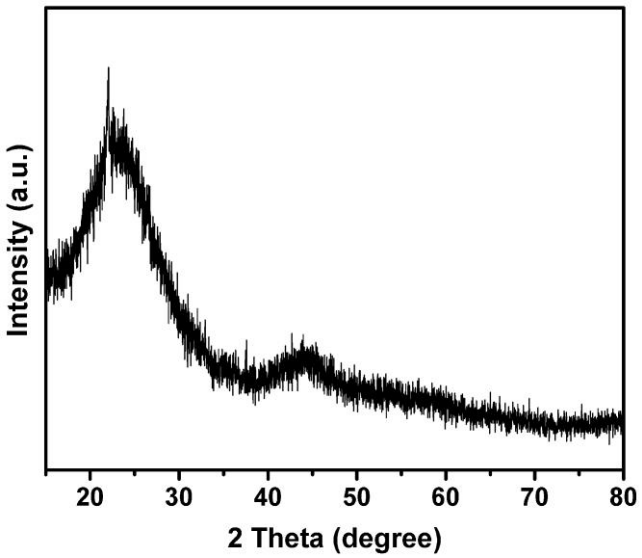

Fig. S3. Powder XRD patterns of the PPN-4/C600-Si.

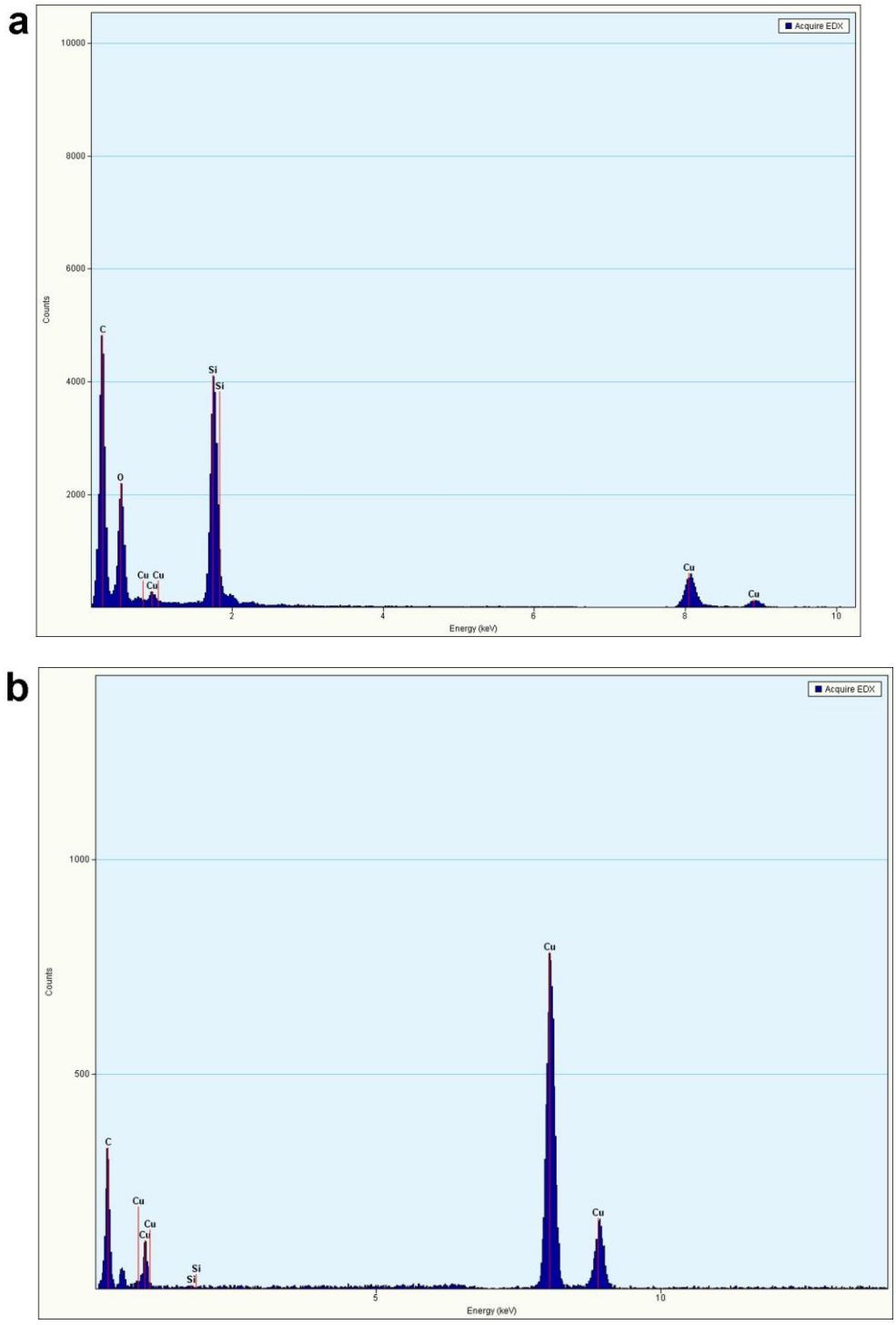

Fig. S4. The comparison of EDS analysis of PPN-4/C600-Si (a) and PPN-4/C600 (b).

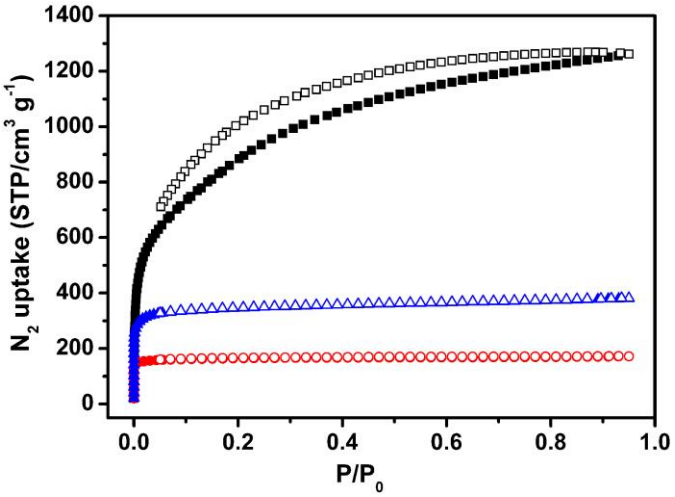

Fig. S5. N_2 sorption isotherms for PPN-4, PPN-4/C600-Si and PPN-4/C600. (adsorption: filled; desorption: open; PPN-4: black squares; PPN-4/C600-Si: red circles; PPN-4/C600: blue triangles).

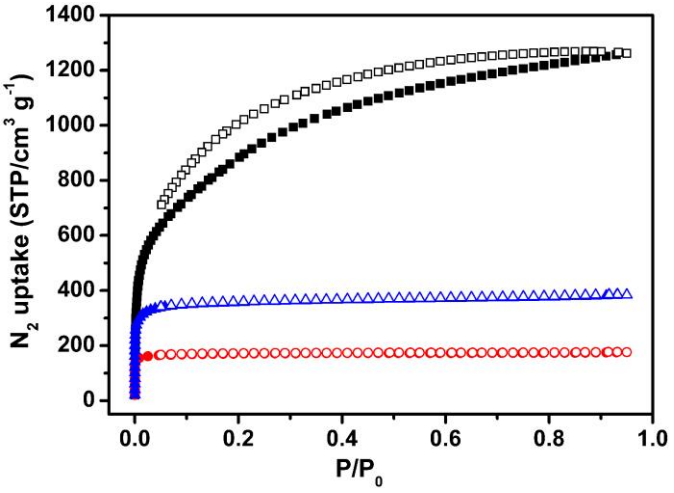

Fig. S6. N_2 sorption isotherms for PPN-4, PPN-4/C800-Si and PPN-4/C800. (adsorption: filled; desorption: open; PPN-4: black squares; PPN-4/C800-Si: red circles; PPN-4/C800: blue triangles).

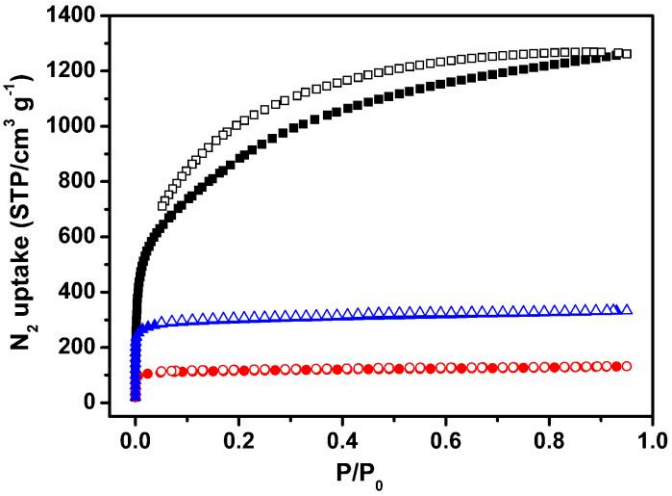

Fig. S7. N_2 sorption isotherms for PPN-4, PPN-4/C1000-Si and PPN-4/C1000. (adsorption: filled; desorption: open; PPN-4: black squares; PPN-4/C1000-Si: red circles; PPN-4/C1000: blue triangles).

Table S1 Surface areas/pore sizes of PPN-4 and carbonized samples

Sample	S_{BET}[a] (m^2 g^{-1})	Pore size[b] (nm)
PPN-4	2882	12.7
PPN-4/C600-Si	636	5.0
PPN-4/C600	1323	4.7
PPN-4/C800-Si	662	5.2
PPN-4/C800	1373	4.8
PPN-4/C1000-Si	443	5.2
PPN-4/C1000	1152	4.8

[a] S_{BET} was calculated in the partial pressure (P/P_0) range of 0.01 to 0.1 which gives the best linearization.

[b] Maxima of the pore size distributions calculated using the Horvath-Kawazoe (HK) model for microporous carbon and DFT model for PPN-4.

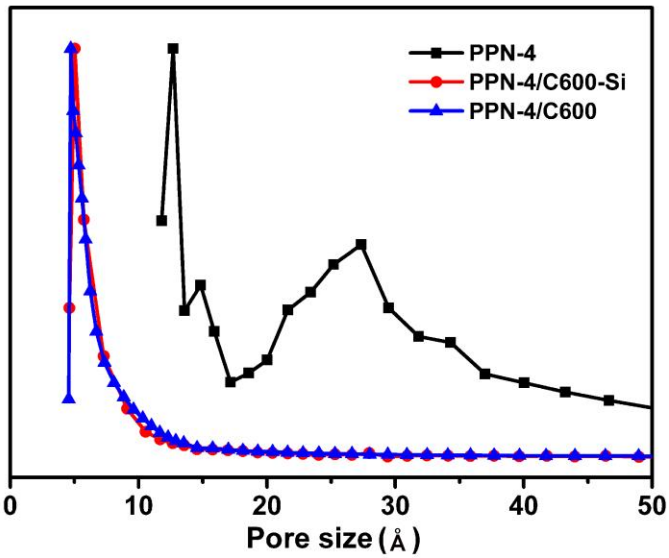

Fig. S8. Pore size distributions for PPN-4, PPN-4/C600-Si and PPN-4/C600.

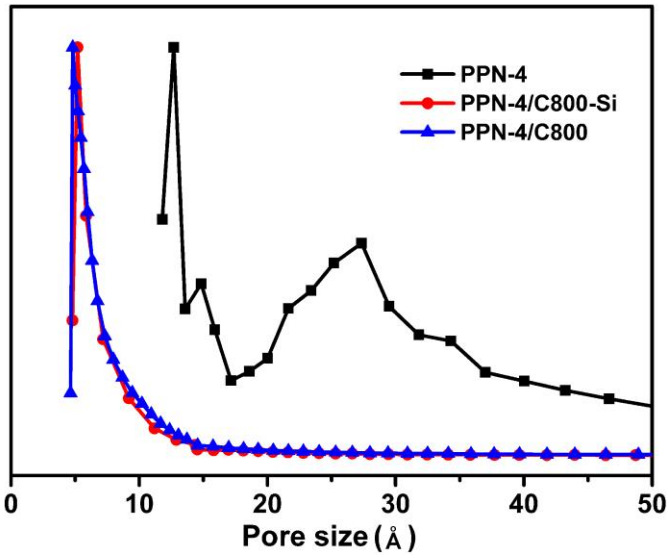

Fig. S9. Pore size distributions for PPN-4, PPN-4/C800-Si and PPN-4/C800.

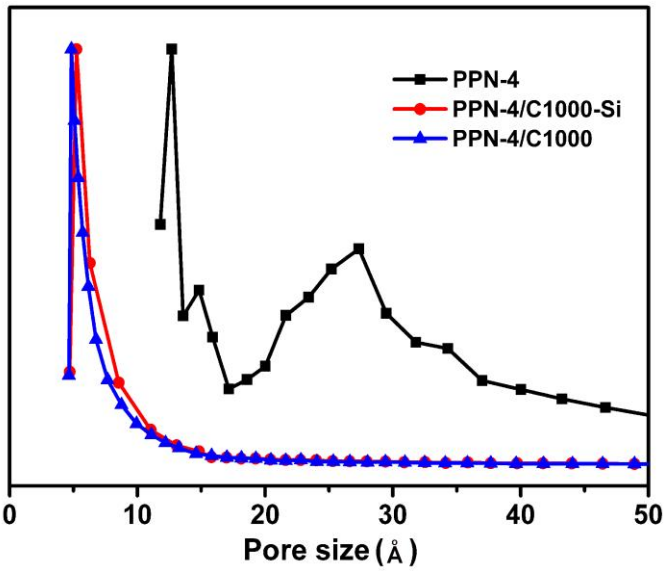

Fig. S10. Pore size distributions for PPN-4, PPN-4/C1000-Si and PPN-4/C1000.

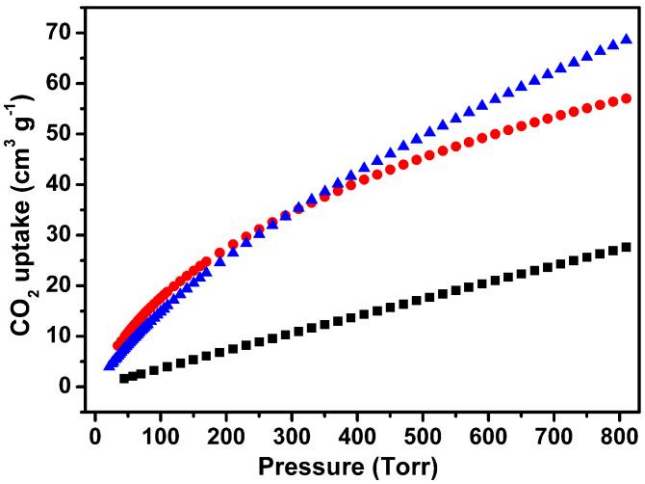

Fig. S11. CO_2 adsorption isotherms of PPN-4, PPN-4/C800-Si and PPN-4/800 at 298 K. (PPN-4: black squares; PPN-4/C800-Si: red circles; PPN-4/C800: blue triangle)

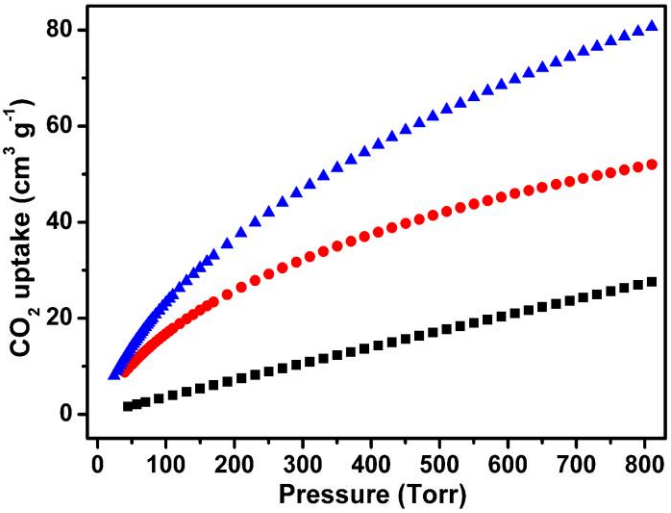

Fig. S12. CO_2 adsorption isotherms of PPN-4, PPN-4/C1000-Si and PPN-4/C1000 at 298 K. (PPN-4: black squares; PPN-4/C1000-Si: red circles; PPN-4/C1000: blue triangle).

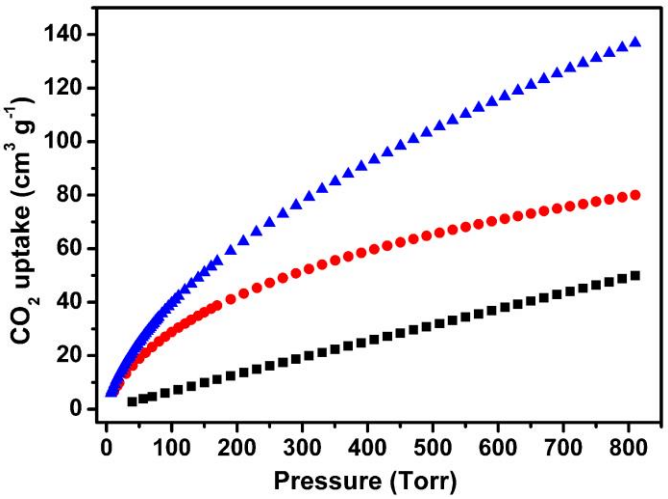

Fig. S13. CO_2 adsorption isotherms of PPN-4, PPN-4/C600-Si and PPN-4/C600 at 273 K. (PPN-4: black squares; PPN-4/C600-Si: red circles; PPN-4/C600: blue triangle).

References

(1) M. Wander, P. J. C. Hausoul, L. A. J. M. Sliedregt, B. J. van Steen, G. van Koten and R. J. M. Klein Gebbink, *Organometallics*, 2009, **28**, 4406.

(2) D. Yuan, W. Lu, D. Zhao and H.-C. Zhou, *Adv. Mater.*, 2011, **23**, 3723.