Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Controllable Nitrogen-Doping of Nanoporous Carbons Enabled by Coordination Frameworks

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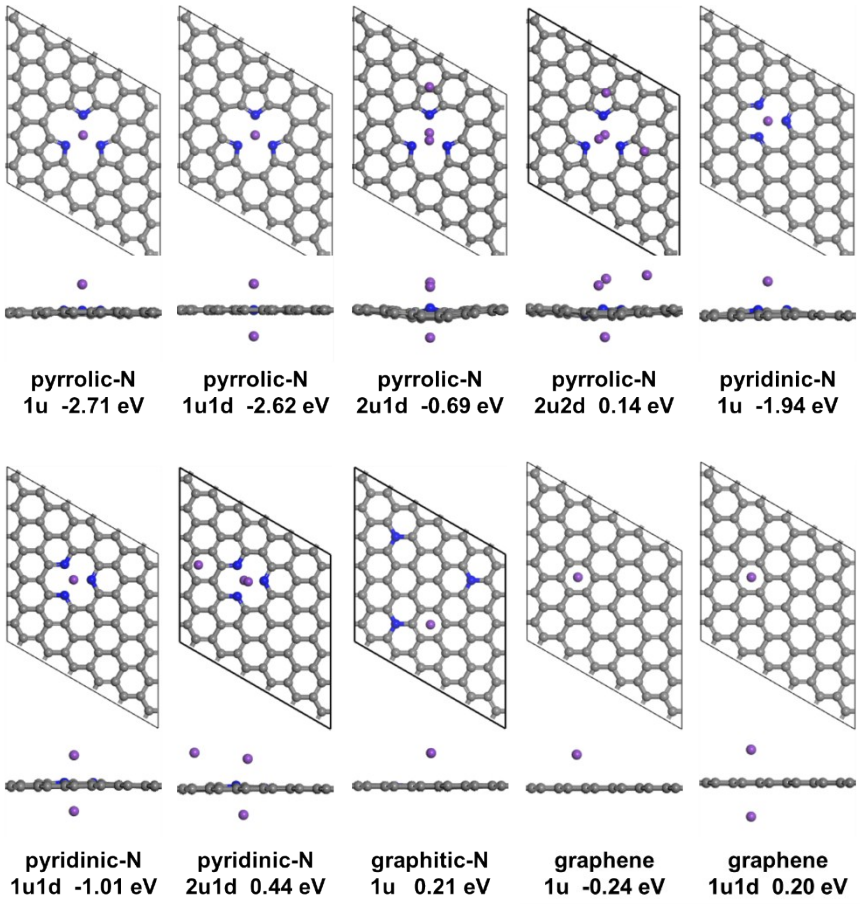

Figure S1. Illustration of pyrrolic-N, pyridinic-N and graphitic-N structures adsorbed by different K atoms. u means that K atoms are adsorbed above the structure, d means that K atoms are adsorbed below the structure. We defined the differential binding energy as $E_{bind}^{diff} = E_{nK/sub} - E_{(n-1)K/sub} - E_K$.[1] Where, n is the number of K atoms, $E_{nK/sub}$ is the total energy of the N-doped carbon structure with adsorbed n K atoms, $E_{(n-1)K/sub}$ is the total energy of the N-doped carbon structure with adsorbed n-1 K atoms, and E_K is the energy of a K atom in the bulk K.

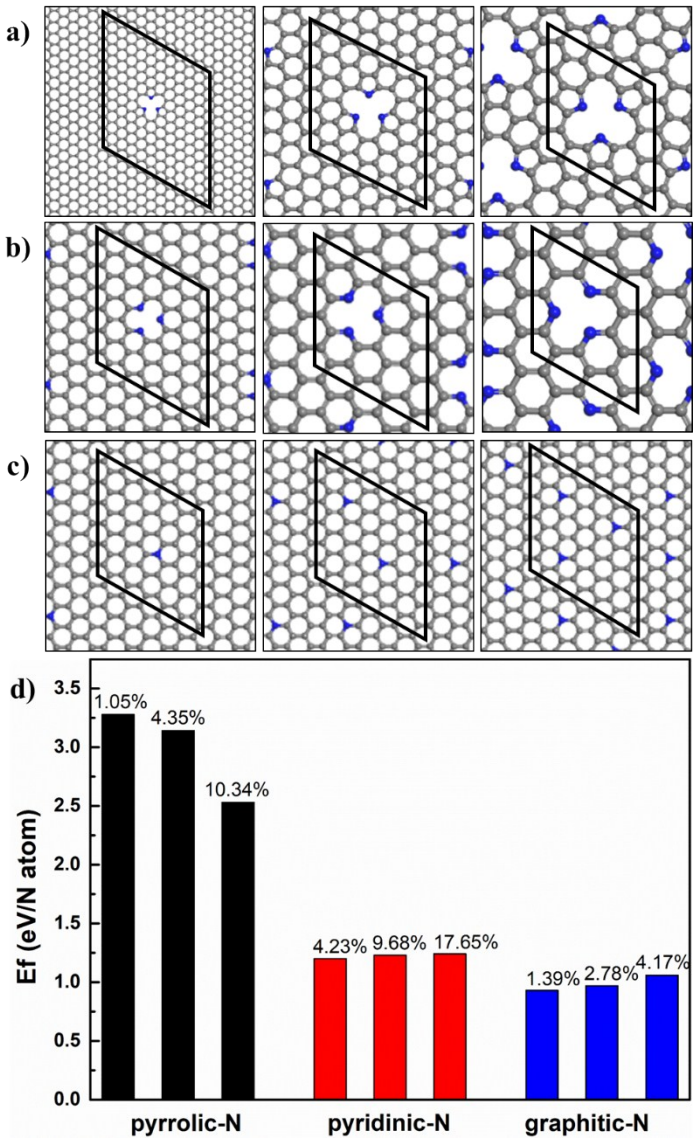

Figure S2. Illustration of pyrrolic-N, pyridinic-N and graphitic-N structures at different N concentrations. (atomic ratio) (a) pyrrolic-N: 1.05%, 4.35% and 10.34%; (b) pyridinic-N: 4.23%, 9.68% and 17.65%; (c) graphitic-N: 1.39%, 2.78% and 4.17%; (d) Formation energies of different N doping structures.

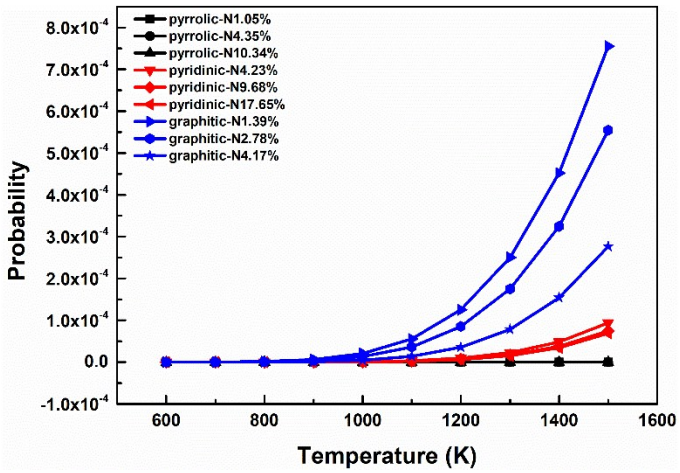

Figure S3. The population probability of pyrrolic-N, pyridinic-N and graphitic-N with different nitrogen concentration versus to the increase of temperature.

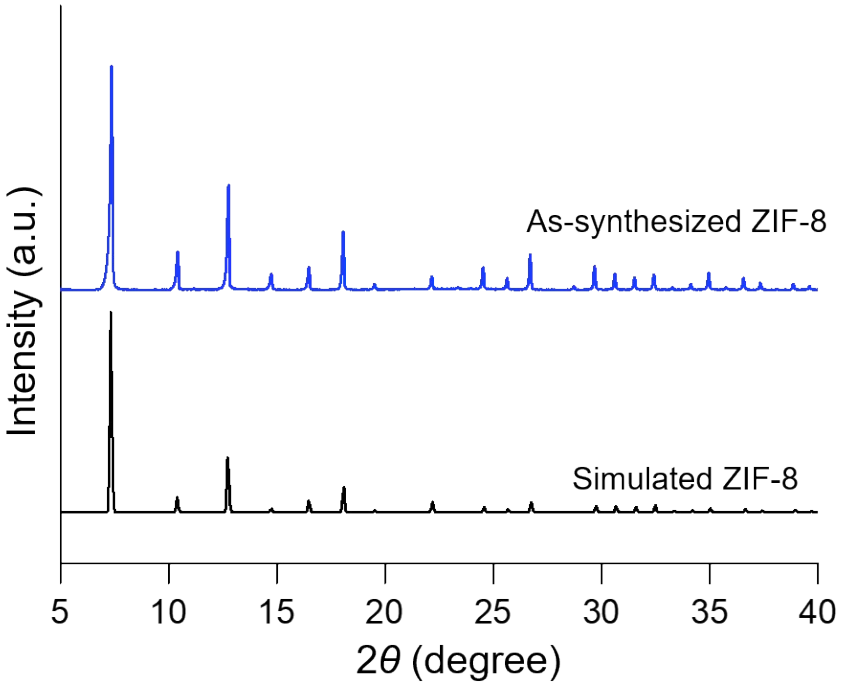

Figure S4. PXRD pattern of the as-synthesized ZIF-8 particles.

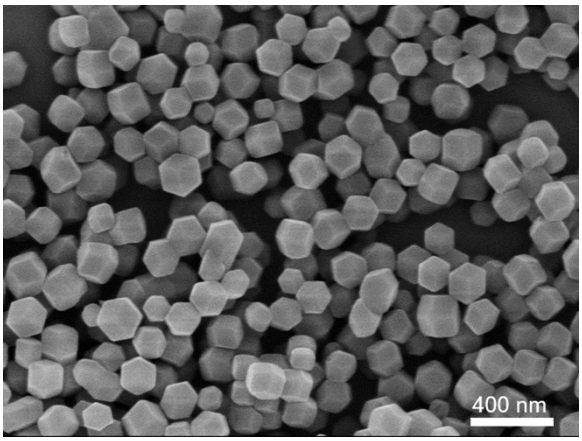

Figure S5. SEM image of the as-synthesized ZIF-8 particles.

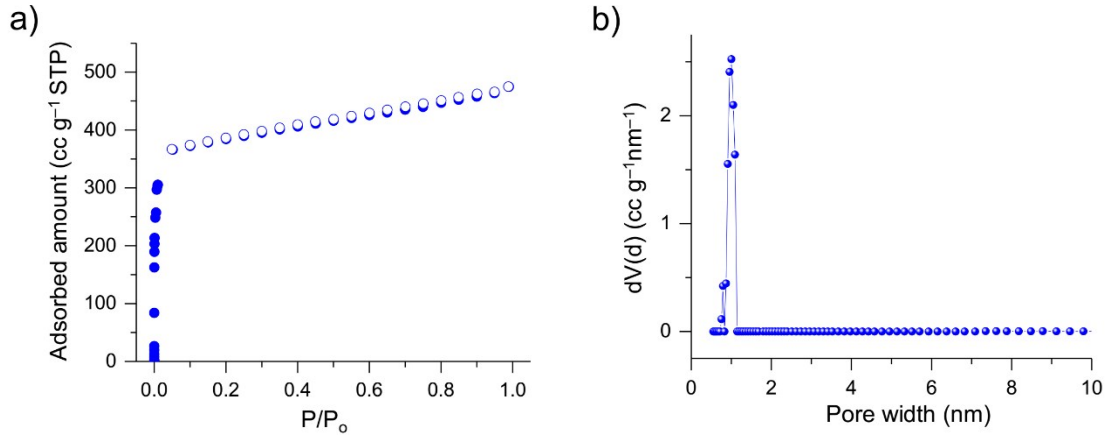

Figure S6. (a) N_2 adsorption-desorption isotherms and (b) the pore size distribution of ZIF-8 precursor.

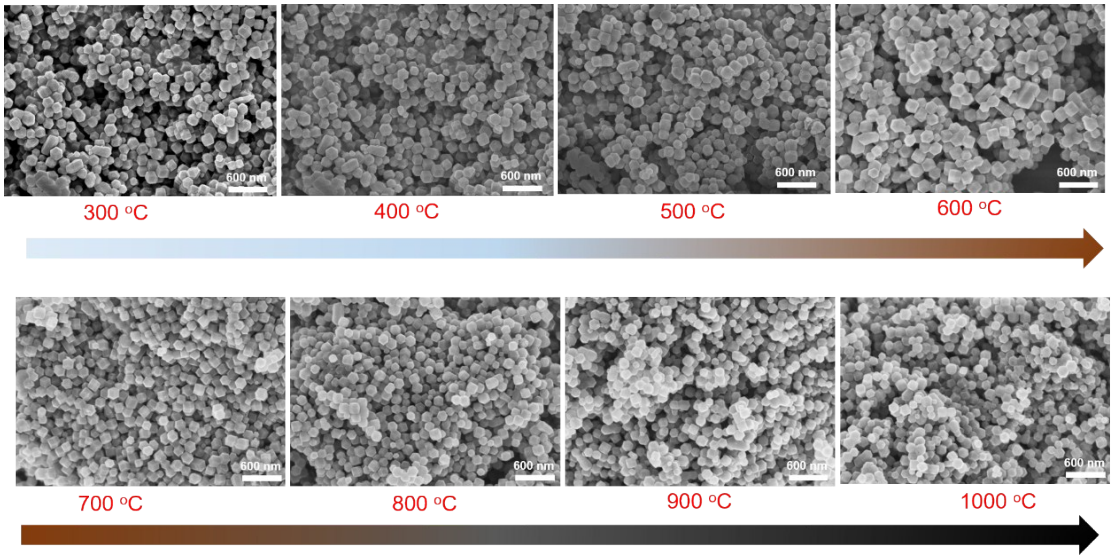

Figure S7. SEM images of the samples obtained by annealing the ZIF-8 particles at various temperatures.

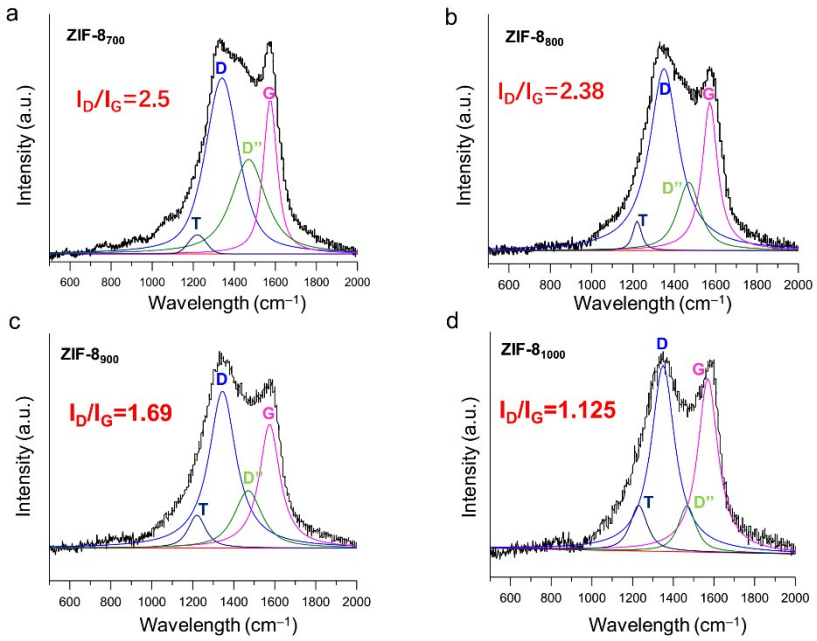

Figure S8. Raman spectra of (a) ZIF-8_{700}, (b) ZIF-8_{800}, (c) ZIF-8_{900} and (d) ZIF-8_{1000}.

The spectra were fitted based on the literature.[2]

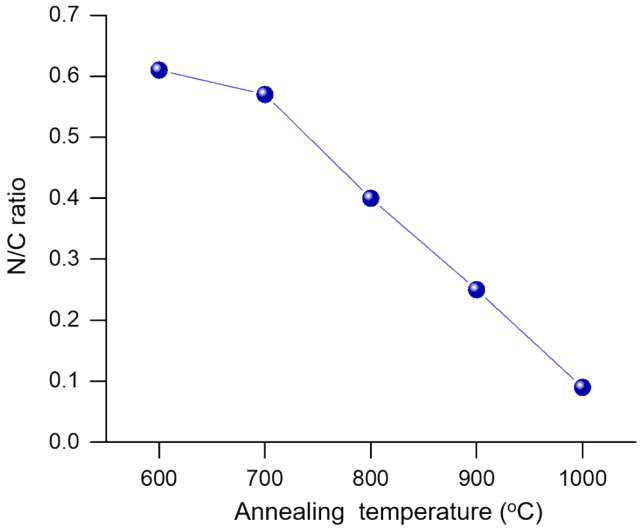

Figure S9. The N/C ratios of all the nanoporous carbons obtained at annealing temperature of 600 to 1000 °C.

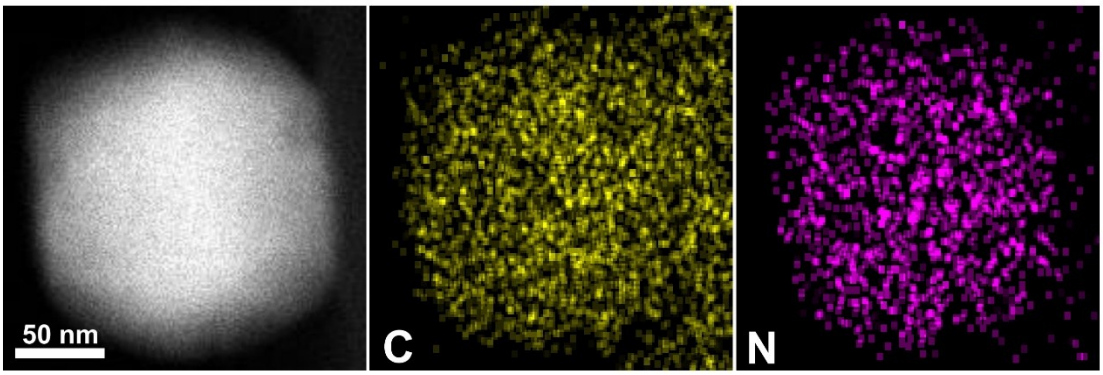

Figure S10. Elemental mapping of the carbonized sample (ZIF-8_{800}).

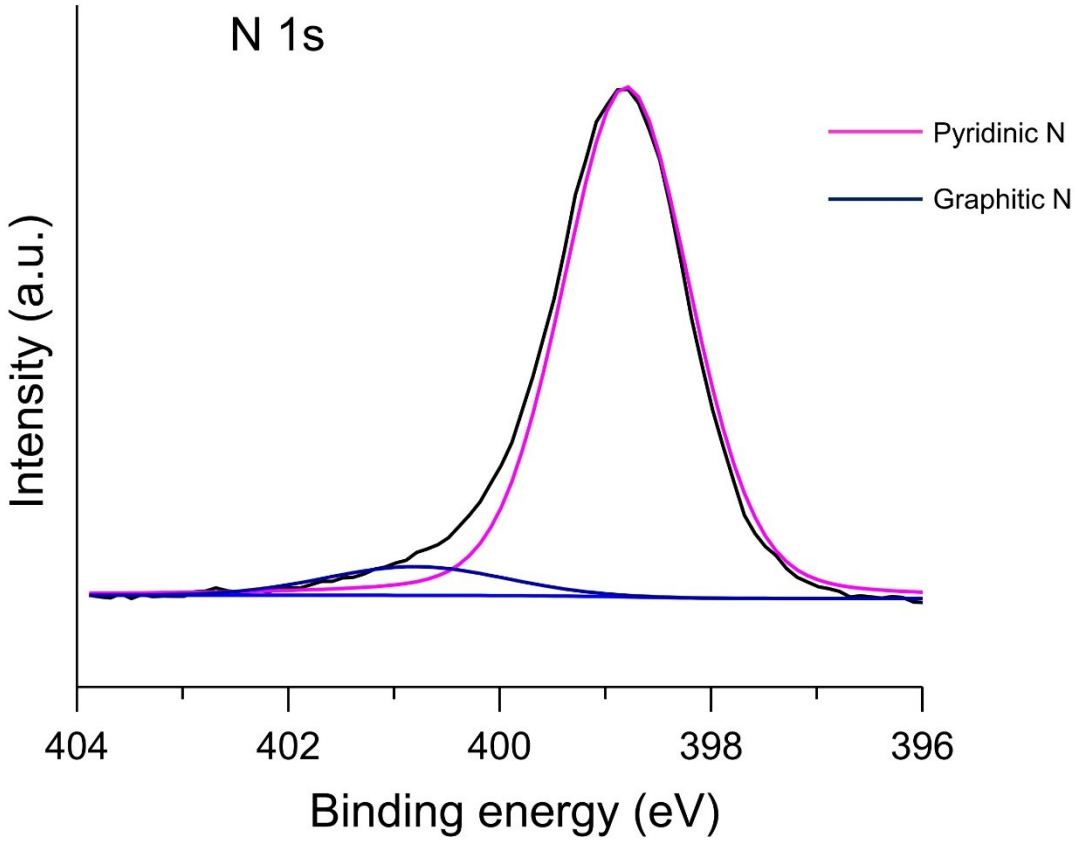

Figure S11. N1s spectra of the sample obtained by annealing the ZIF-8 particles at 700 ^{o}C for 12 h.

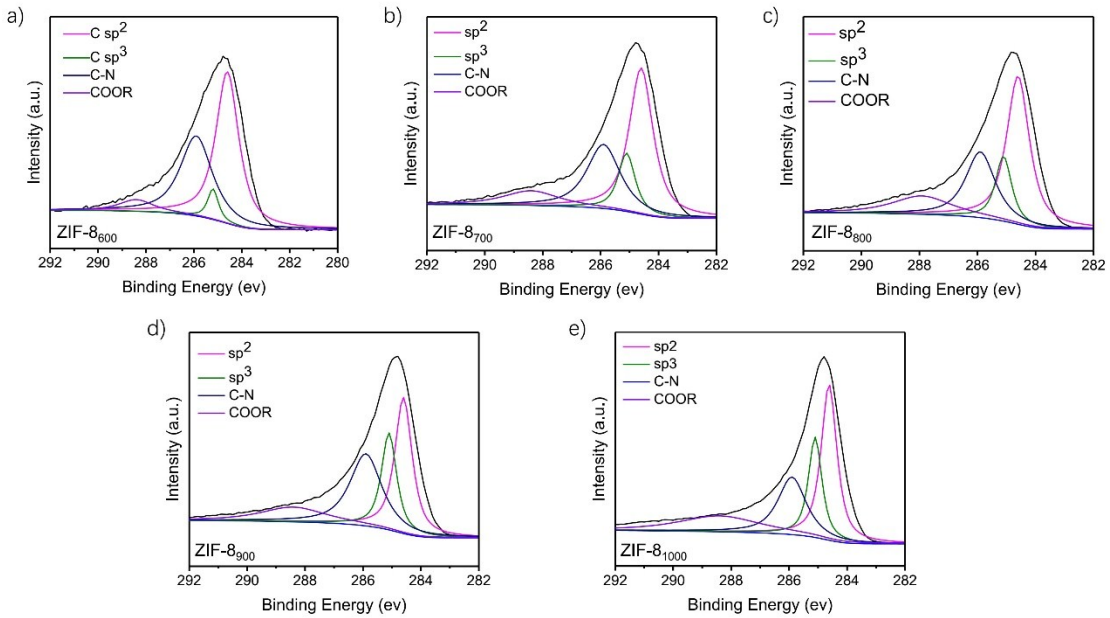

Figure S12. C1s spectra of the samples obtained by annealing the ZIF-8 particles at various temperatures.

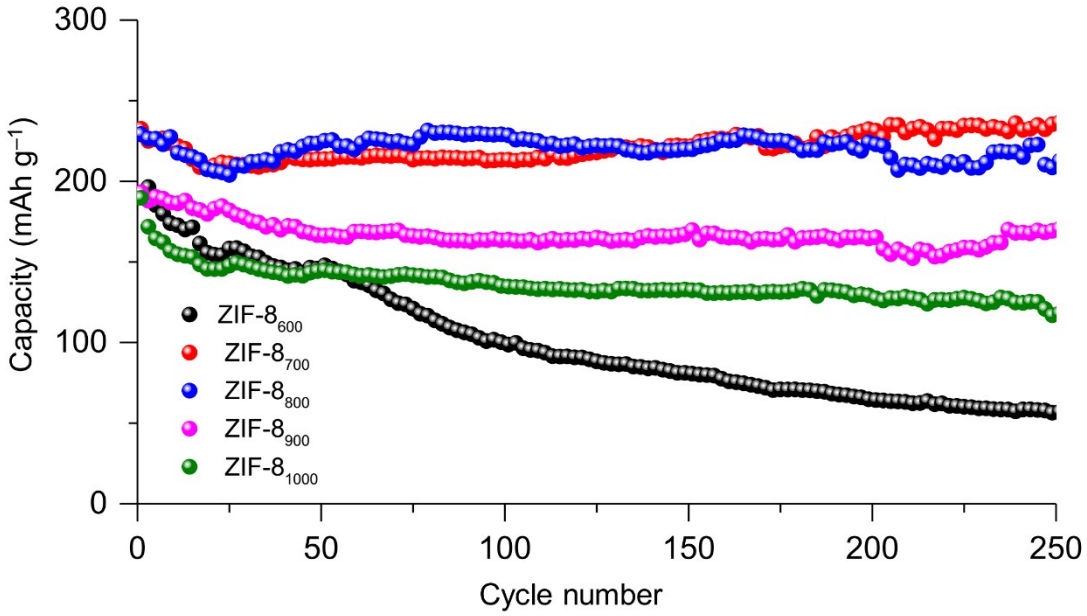

Figure S13. Cycling performance of ZIF-8 carbonized under temperatures ranging from 600 ^{o}C to 1000 ^{o}C with a current of 30 mA g^{-1}.

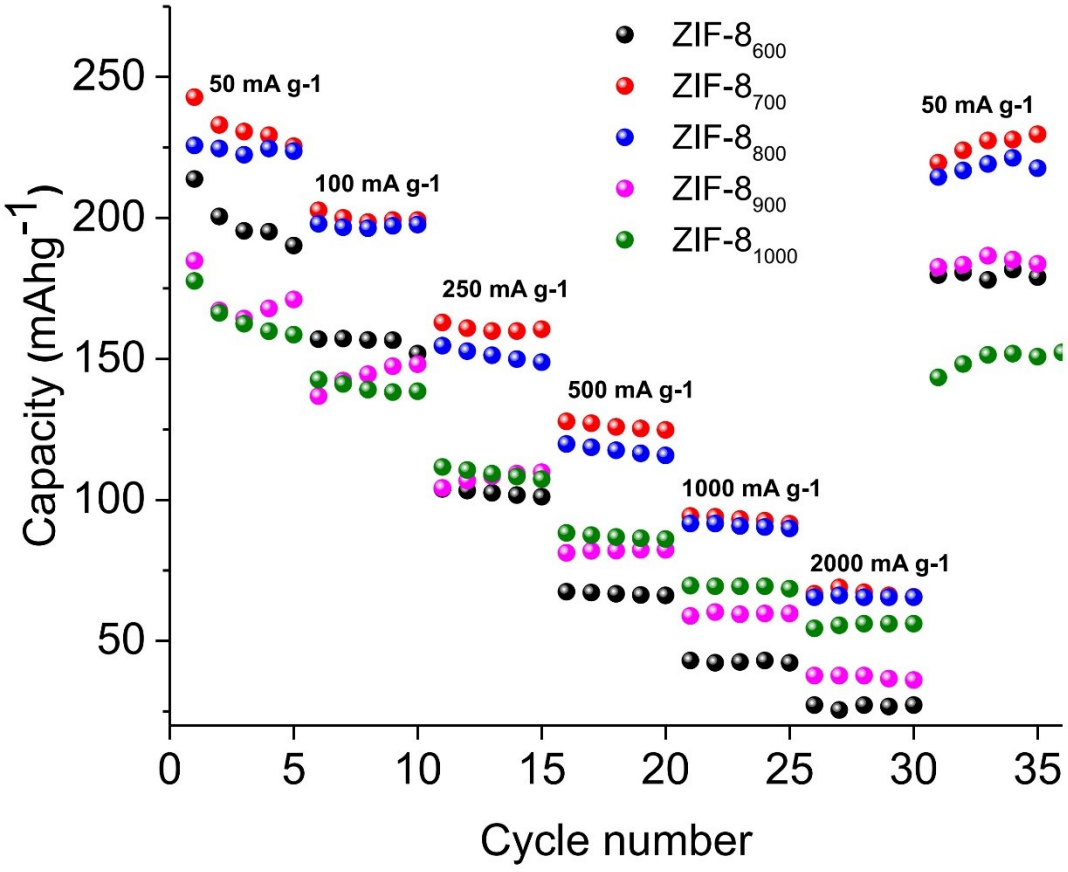

Figure S14. Rate performance of the ZIF-8 carbonized under various temperatures ranging from 600 °C to 1000 °C with various current density from 50 to 2000 mA g^{-1}.

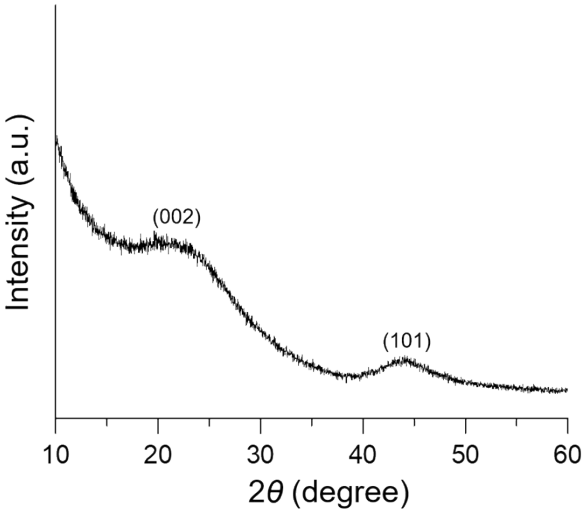

Figure S15. PXRD pattern of the hard carbon.

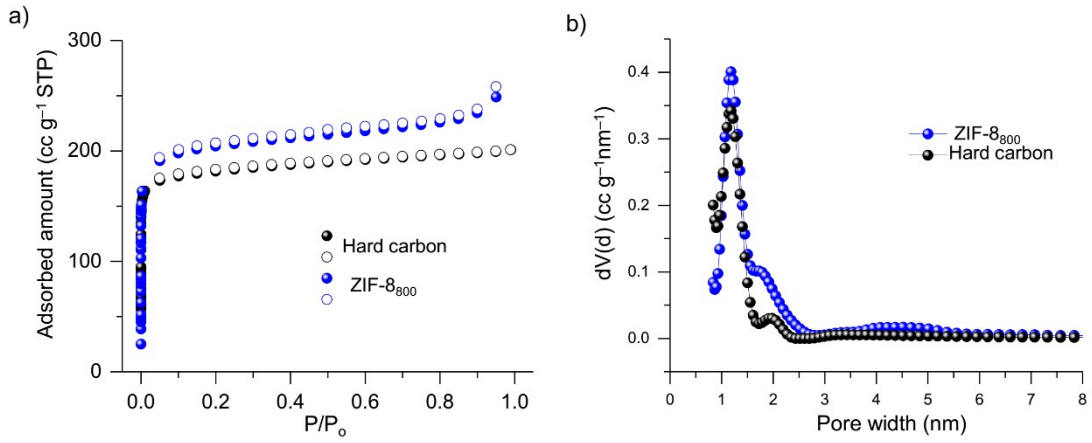

Figure S16. (a) N_2 adsorption-desorption isotherms and (b) the pore size distribution of ZIF-8_{800} and hard carbon.

Table S1. Comparison of cycling performance of various carbon-based anodes.

Materials	Capacity Retention (mAh g^{-1})	Remaining capacity (cycles)	Current Density (mA g^{-1})	References
ZIF-8_{800}	220	100% (100)	100	This work
Graphite	97	51% (50)	139	Ref. S3
Soft carbon	162	81% (50)	558	Ref. S3
Hard carbon	216	83% (100)	28	Ref. S4
N-graphene	210	78% (100)	100	Ref. S5
Polynanocrystalline Graphite	75	50 % (300)	100	Ref. S6
HCNT	232	100% (50)	100	Ref. S7
Mesoporous Carbon	198	90% (200)	200	Ref. S8
HCS-SC	186	90% (200)	279	Ref. S9

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