Supporting Information

Rational Design of Covalent Triazine Frameworks Based on Pore Size and Heteroatomic toward High Performance Supercapacitors

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Content

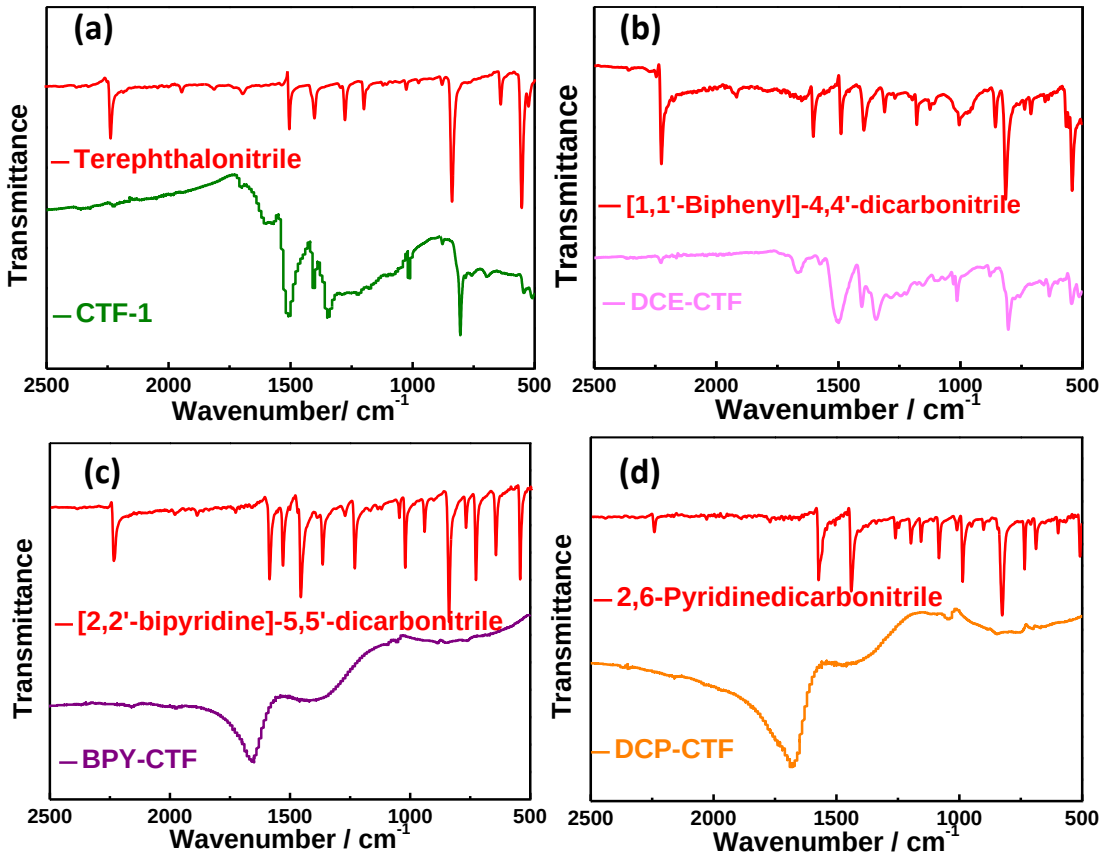


Fig. S1. FT-IR spectra of terephthalonitrile, [1,1'-biphenyl]-4,4'-dicarbonitrile, [2,2'-bipyridine]-5,5'-dicarbonitrile, pyridine-2,6-dicarbonitrile, CTF-1, DCE-CTF, BPY-CTF and DCP-CTF.

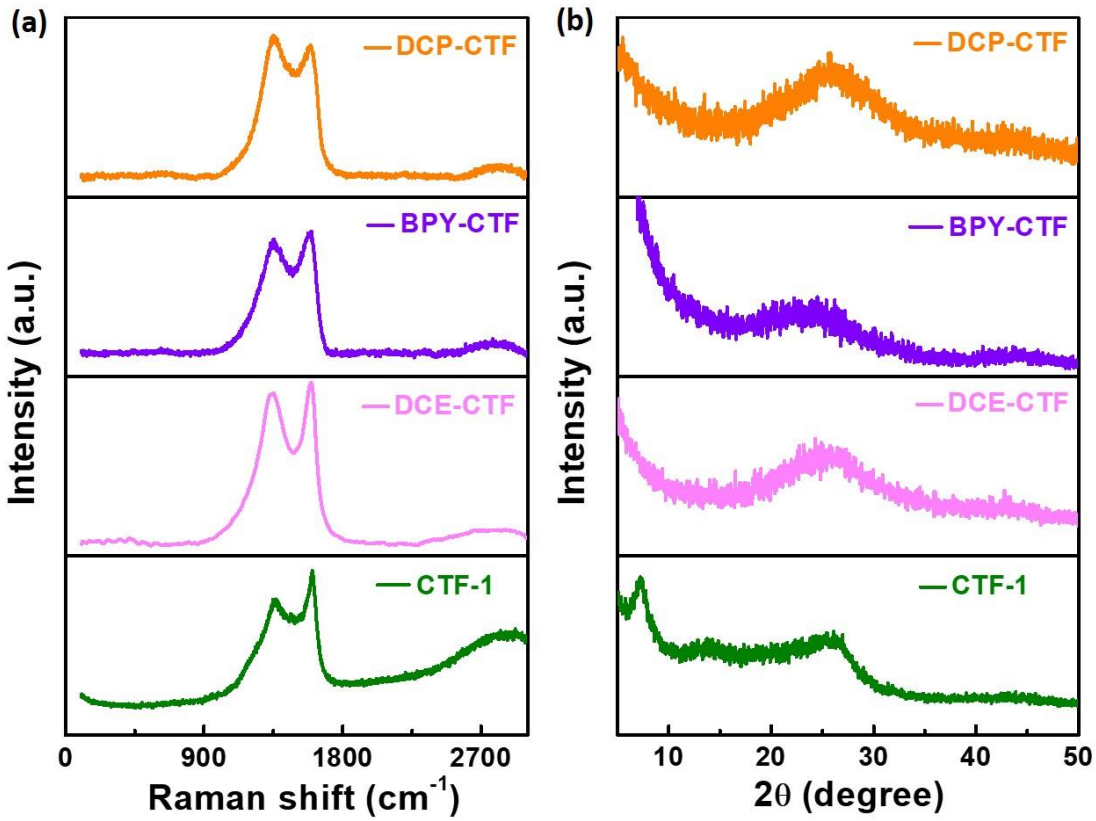


Fig. S2. (a) The Raman spectra and (b) XRD patterns of CTF-1, DCE-CTF, BPY-CTF and DCP-CTF.

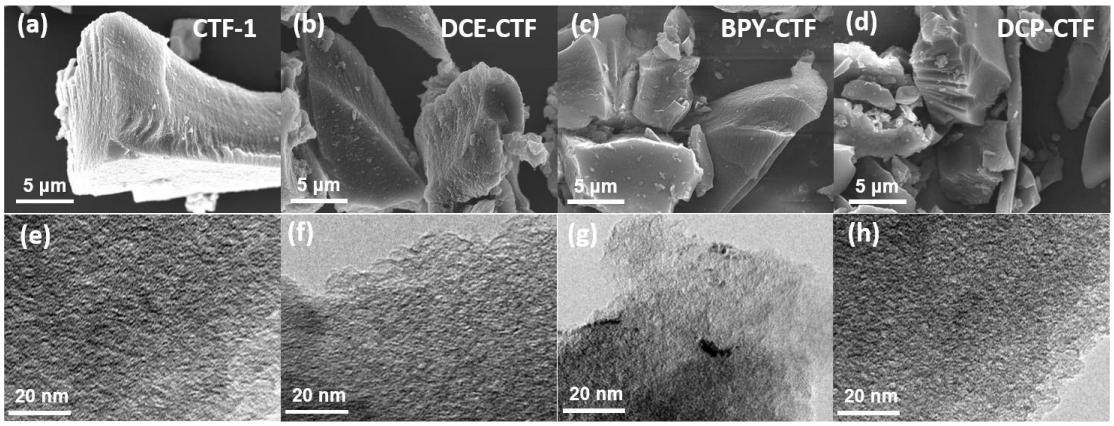
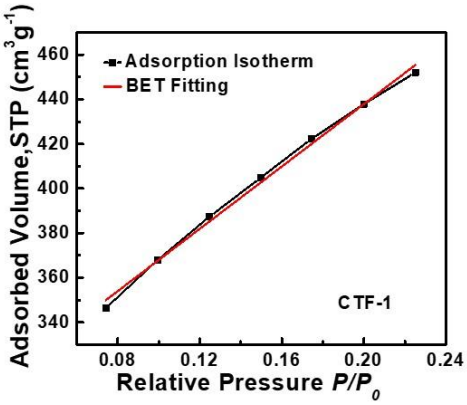
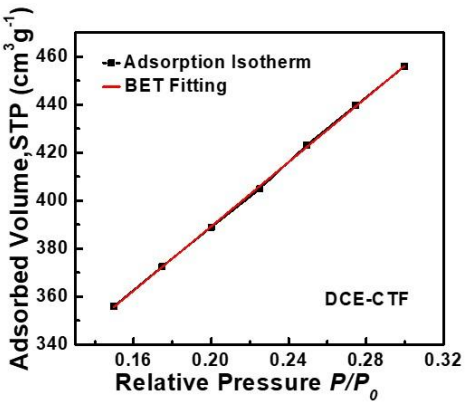


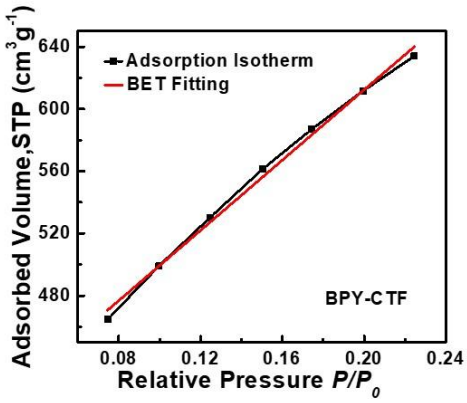
Fig. S3. (a)–(d) The SEM images and (e)–(h) the TEM images of CTF-1, DCE-CTF, BPY-CTF and DCP-CTF.



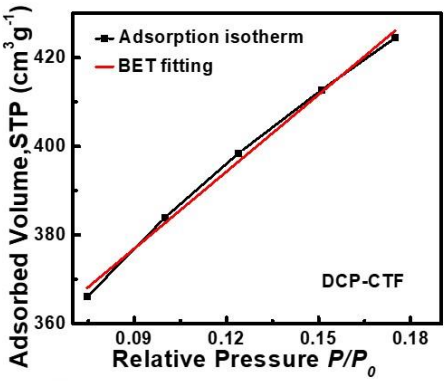
Slope = 2.170
Intercept = 2.368e-02
Correlation coefficient, r = 0.999945
C constant= 92.619
Surface Area = 1587.681 m^2g^{-1}



Slope = 2.357
Intercept = 4.265e-02
Correlation coefficient, r = 0.999936
C constant= 56.269
Surface Area = 1451.199 m^2g^{-1}



Slope = 1.501
Intercept = 2.707e-02
Correlation coefficient, r = 0.999947
C constant= 56.470
Surface Area = 2278.290 $m^2\ g^{-1}$



Slope = 1.537
Intercept = 2.463e-02
Correlation coefficient, r = 0.999970
C constant= 63.420
Surface Area = 2229.773 $m^2\ g^{-1}$

Fig. S4. N_2 adsorption–desorption isotherms and the calculated pore parameters of CTF-1, DEC-CTF, BPY-CTF, and DCP-CTF.

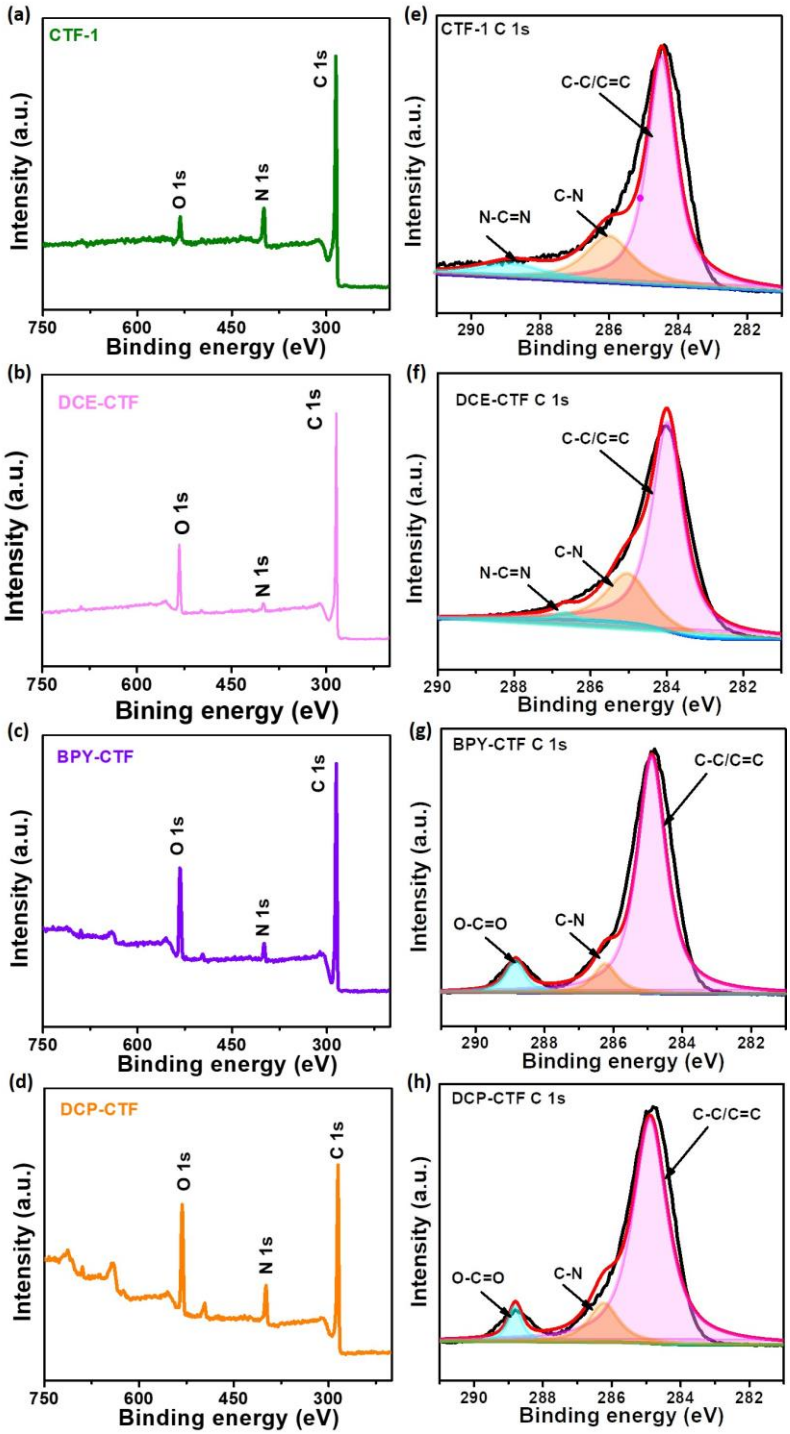


Fig. S5. The XPS for CTF-1, DCE-CTF BPY-CTF and DCP-CTF.

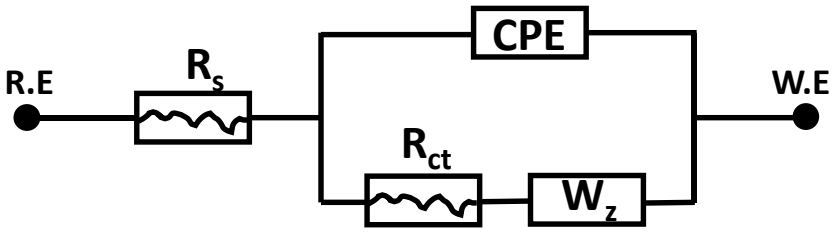


Fig. S6. Equivalent circuit of the impedance spectra.

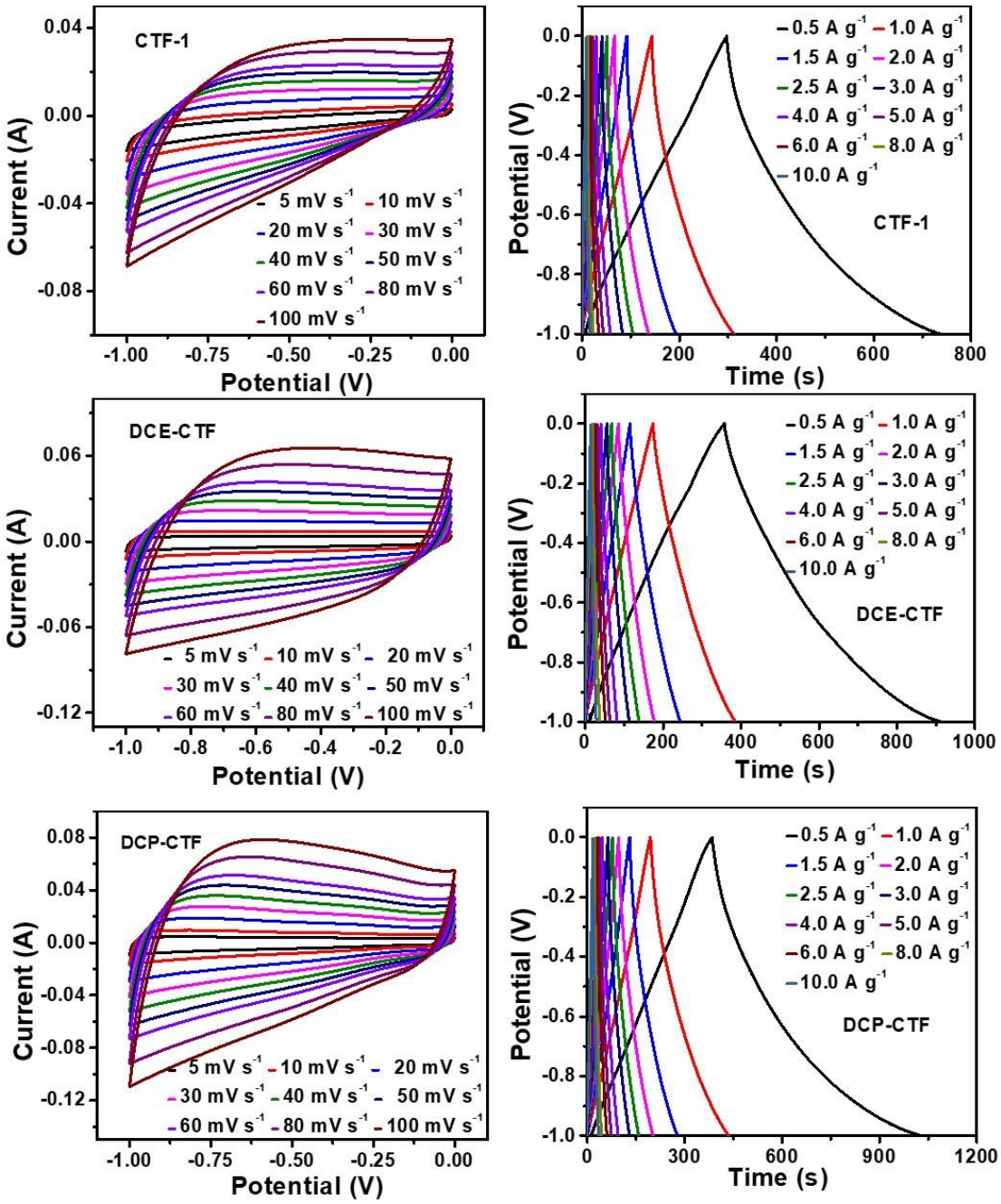


Fig. S7. CV cures and GCD cures of CTF-1, DCE-CTF, and DCP-CTF at different scan rate.

Table S1. BET Surface areas, micropores specific surface area, mesoporous specific surface area, and total pore volume of CTF-1, DCE-CTF, BPY-CTF and DCP-CTF.

Electrode materials	**BET specific surface areas (m^2 g^{-1})**	**Micropores specific surfaces area (m^2 g^{-1})**	**Mesoporous specific surfaces area (m^2 g^{-1})**	**Total Pore Volume (cm^3 g^{-1})**
CTF-1	1558	934	624	0.978
DCE-CTF	1451	0	1451	1.620
BPY-CTF	2278	990	1288	1.485
DCP-CTF	2229	844	1384	1.493

Table S2. Nitrogen contents of CTF-1, DCE-CTF, BPY-CTF and DCP-CTF from XPS.

Electrode materials	Nitrogen contents (%)
CTF-1	11.8
DCE-CTF	4.7
BPY-CTF	11.3
DCP-CTF	13.0

Table S3. Peak areas of three kinds of N-configurations in CTFs, which are got from the deconvolution analysis results of N 1s.

Electrode materials	$\mathbf{N_{pyridinic}}$	$\mathbf{N_{pyrrolic}}$	$\mathbf{N_{quaternary}}$
CTF-1	6695	4030	3014
DCE-CTF	4224	5125	3812
BPY-CTF	11421	10393	10695
DCP-CTF	14546	8423	9933

The ration of $N_x = \frac{N_x}{N_{pyridinic}+N_{pyrrolic}+N_{quaternary}}$

Table S4. Summary of electrochemical performance of CTFs as electrode materials for supercapacitors.

Electrode materials	Electrolytes	Specific capacitance ($F \cdot g^{-1}$)	Ref
PDC-MA-COF	6 M KOH	335@1 $A \cdot g^{-1}$	S1
N-PC	6 M KOH	112@1 $A \cdot g^{-1}$	S2
TPT-DAHQ COF	1 M KOH	256@1 $A \cdot g^{-1}$	S3
TCNQ-CTF-800	1 M KOH	380@0.2 $A \cdot g^{-1}$	S4
TDFP-1	0.1 M H_2SO_4	354@2.0 mV s^{-1}	S5
p-CTF-600	1 M H_2SO_4	340.1@0.2 $A \cdot g^{-1}$	S6
Car-CTFs	1 M KCl	545@5 mV s^{-1}	S7
PTF-700	$EMIMBF_4$	151.3@0.1 $A \cdot g^{-1}$	S8
G-PCs	6 M KOH	340@0.1 $A \cdot g^{-1}$	S9
FUM-700	6 M KOH	400@1 $A \cdot g^{-1}$	S10
LNU-18-800	6 M KOH	269@0.5 $A \cdot g^{-1}$	S11
AC-900	6 M KOH	278@1 $A \cdot g^{-1}$	S12
TPDA-1	1 M H_2SO_4	469.4 F@2 mV s^{-1}	S13
FCTF	1 M H_2SO_4	379@1 $A \cdot g^{-1}$	S14
DCP-CTF-700	2.96 M $ZnCl_2$	154@1 $A \cdot g^{-1}$	S15
BPY-CTF	**1 M KOH**	**393.6@0.5 A g^{-1}**	**This work**

Table S5. DFT specific surface areas and specific surface areas derived from micropores and mesopores of CTF-1, DCE-CTF, BPY-CTF and DCP-CTF.

DFT SSA / Materials	DFT SSA $m^2 g^{-1}$	Micropores SSA $m^2 g^{-1}$	Mesopores SSA $m^2 g^{-1}$
CTF-1	1220	951	269
DCE-CTF	1080	518	562
BPY-CTF	1640	1210	430
DCP-CTF	1660	1240	420

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