

Supporting Information

Novel synthetic approach for designing metal free, redox active quinoxaline-benzimidazole based organic polymers with high energy storage capacity.

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Section S-1:

Experimental

M-cresol, selenium dioxide and dichloromethane (s. d. fine Bombay) were purified. Phenylacetyl chloride, biphenyl dicarboxylic acid (BPDA) and 3, 3' Diamino benzidine (Sigma Aldrich) were used as received. The inherent viscosities of QOP and QOP-BOP were measured with 3 % concentration in m-cresol at 30 °C using Ubbelohde suspended level viscometer. The chemical structure of intermediates, monomer and polymers were recorded on a Thermo Nicoletis-10 Mid Fourier transform infrared spectrometer. Proton NMR of monomer and polymer were obtained with a Bruker spectrophotometer. X-ray diffraction of polymers was recorded on Rigaku X-ray Diffraction System. Thermogravimetric analysis was performed on a Mettler Toledo Thermal Analysis system under nitrogen atmosphere with a scan rate of 10°C min⁻¹. Differential Scanning Calorimetry was performed on a Mettler Toledo DSC at a heating rate of 10°C min⁻¹. The scanning electron micrograph of the sample was taken with the help of JSM5910 Scanning Electron Microscope, JEOL, Japan. Cyclic Voltammogram measurements was carried out with a CHI 608E Electrochemical Analyzer (CH Instruments Inc., USA) with polymer coated on stainless steel plate was taken as anode, platinum wire as cathode and the reference electrode was a saturated calomel electrode. Experiments were performed in 1M Na₂SO₄ solutions as an electrolyte and measured at a potential scan rate of 2-100mV/s.

Section S-2:

¹H NMR of Polymer

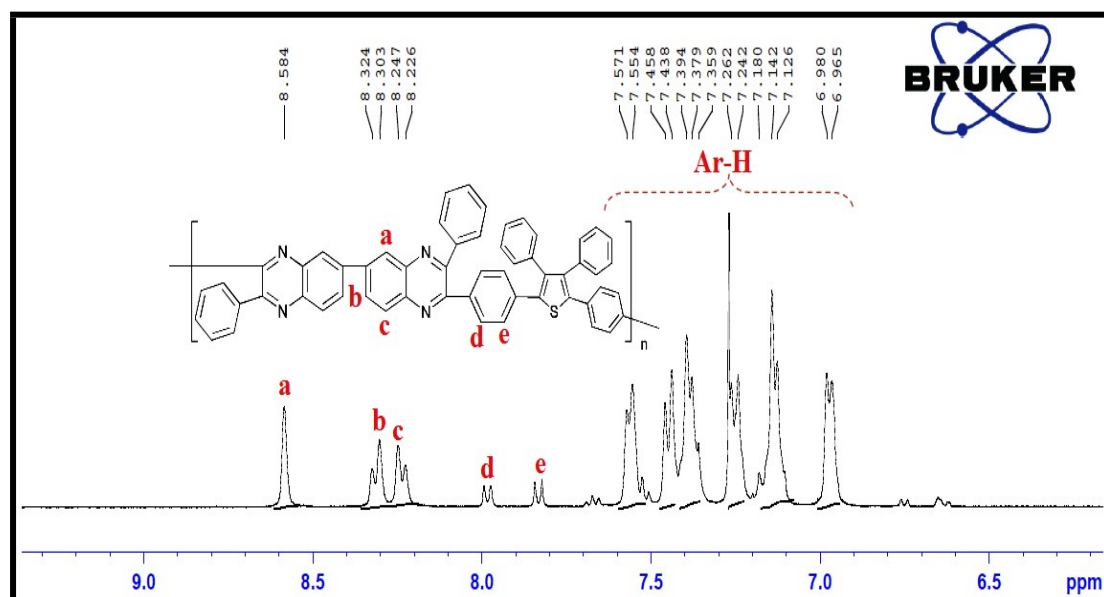


Figure S-1: ¹H NMR of QOP.

Section S-3: Energy Dispersive X-ray Spectroscopy (EDX)

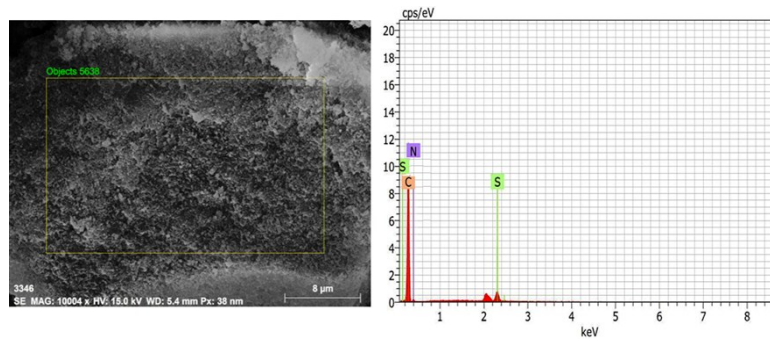


Figure S-2: Energy Dispersive X-ray Spectroscopy (EDX) of copolymer QOP-BOP.

Section S-4: Electrochemical Analysis

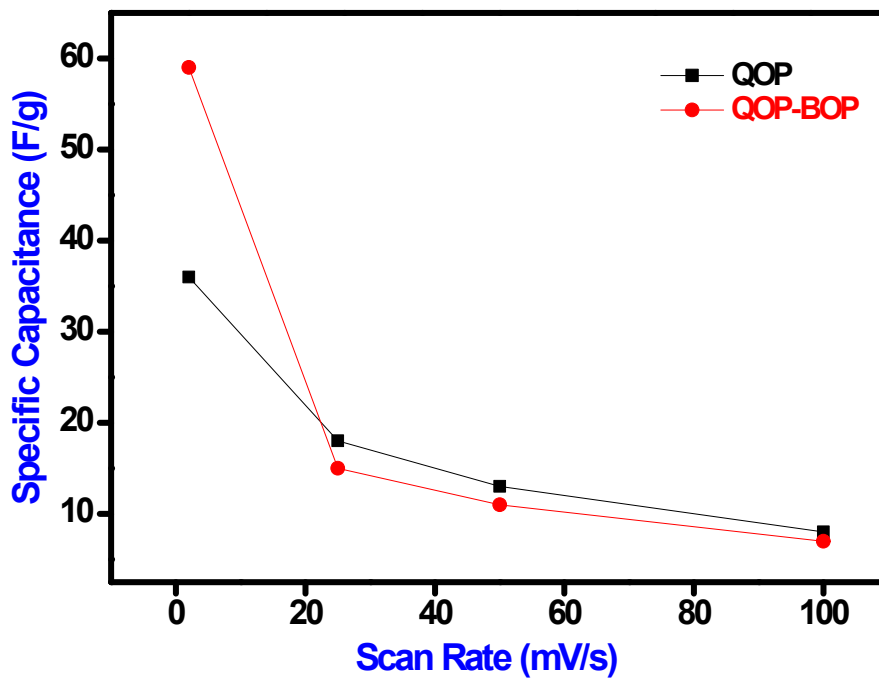


Figure S-3: Variation of scan rate Vs specific capacitance.

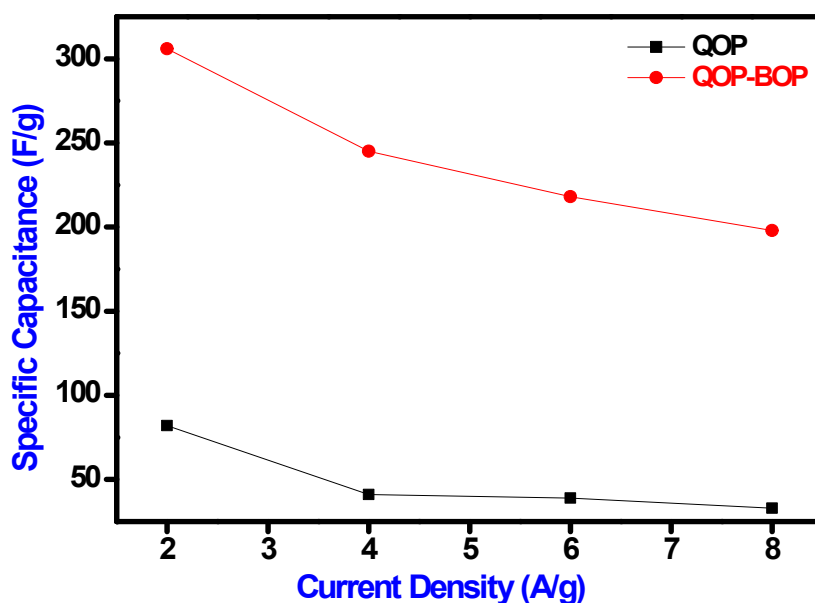


Figure S-5: Variation of current density Vs specific capacitance.

Calculations

The electrical parameters such as specific energy, specific power and columbic efficiency of QOP and QOP-BOP electrodes calculated using following formulae:

$$\text{Specific energy} = V \times I_d \times T_d / W \quad (1)$$

$$\text{Specific power} = V \times I_d / W \quad (2)$$

$$\text{Columbic efficiency } \eta (\%) = T_d / T_c \times 100 \quad (3)$$

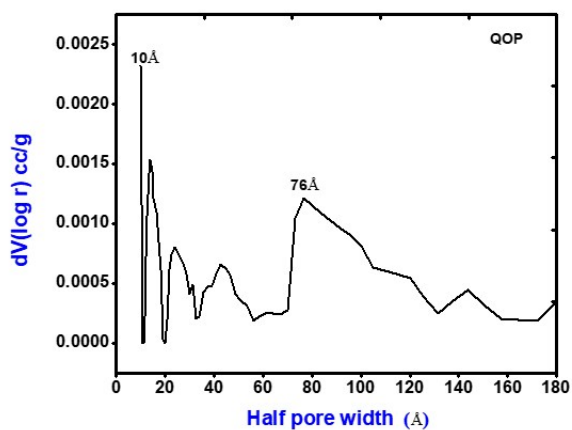
Where, V is the applied potential, W is the mass of electrode dipped in the electrolyte, I_d is discharging current, T_d is discharging time and T_c is charging time. It is found that QOP electrode has the specific energy of 70.90 Wh/kg, specific power of 31.66 KW/kg and columbic efficiency 75 %. Similarly QOP-BOP electrode has the specific energy of 92.40 Wh/kg, specific power of 11.00 KW/kg and columbic efficiency 65 % at 1mA current density in 1M Na_2SO_4 electrolyte solution.

Table S-1. Parameter values by fitting the impedance data of QOP and QOP-BOPfilmt to equivalent circuit shown in main manuscript figure 4.

Parameters	QOP	QOP-BOP
Components		

R	3.406	5.66
Cdl/mFg ⁻¹	2.01x10 ⁻⁴	2.04x10 ⁻⁴
R ₁ /k.ohm	233.2	256.2
R ₂ /k.ohm	1228	1244
W/mS s ⁻ⁿ	0.00139	0.00152
CPE	2.99X10 ⁻⁴	2.99X10 ⁻⁴

Section S-5. NLDFIT study of QOP and QOP-BOP



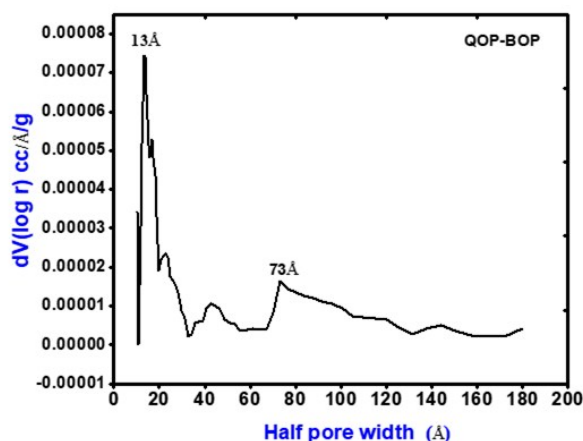
DFT method summary

Pore volume = 0.100 cc/g
 Lower confidence limit = 10.104 Å
 Fitting error = 0.734 %
 Half pore width (Mode) = 10.104 Å

Moving point average: off

DFT method summary

Pore volume = 0.100 cc/g
 Lower confidence limit = 10.104 Å
 Fitting error = 0.734 %
 Half pore width (Mode(dLog)) = 76.550 Å



DFT method summary

Pore volume = 0.002 cc/g
 Lower confidence limit = 10.104 Å
 Fitting error = 0.536 %
 Half pore width (Mode) = 13.236 Å

Moving point average: off

DFT method summary

Pore volume = 0.002 cc/g
 Lower confidence limit = 10.104 Å
 Fitting error = 0.536 %
 Half pore width (Mode(dLog)) = 73.182 Å

Moving point average: off

Figure S-6: Pore size distribution curve for QOP and QOP-BOP derived from N₂ adsorption isotherm at 77 K using the NLDFT method.

Section S-6. Comparative study of electrochemical charge storage activity of different electrode materials

Table S-2.

Electrode Material	Electrolyte	Specific capacitance (F/ g)	Current density (A g ⁻¹)	Reference
azo based covalent organic frameworks (COFs)	1 M Na ₂ SO ₄	226		1
Porous triazine-based frameworks (PTF)	1-ethyl-3-methylimidazolium Tetrafluoroborate	147 (PTF@500°C) 151(PTF@700 °C)	0.1	2
Graphene	30 wt.% KOH	150	0.1	3
Radical COFs (i)[TEMPO]100 %-NiP-COF (ii) [TEMPO]50%-NiP-COF	0.1 M (C ₄ H ₉) ₄ NCIO ₄ in CH ₃ CN	(i)167 (ii) 124	0.1	4
Hierarchically porous B doped carbons	1 M H ₂ SO ₄	160	10 mV/s	5

Nitrogen-doped porous carbon foam	6 M KOH	210	0.5	6
Hierarchically porous carbon AS-ZC-800	1 M H ₂ SO ₄	251	0.25	7
MOF-derived nonporous carbons	1 M H ₂ SO ₄	251	0.5	8
Interconnected micropores Carbon	1 M H ₂ SO ₄	258	0.5	9
TpDAB	1M Na ₂ SO ₄	432	0.5	10
PAM	1M NaOH	252	5 mV/s	11
β -ketoenamine-linked conjugated microporous polymer	1M H ₂ SO ₄	252	1	12
Reduced graphene oxide hydrogels	1 M H ₂ SO ₄ + 0.2 M HQ	252.6	1	13
N-rich hollow carbon sphere	5 M KOH	230	0.5	14
MnO ₂ /CNT	1 M Na ₂ SO ₄	201	1	15
QOP-BOP	1M Na₂SO₄	305	2	Present Work

Section S-7.

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