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Electronic Supplementary Information

Para-Azaquinodimethane Integrated Quinoidal Conjugated Microporous Polymer

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Materials and measurements

All chemicals and solvents were purchased from commercial suppliers and used without further purification unless otherwise specified. ^{13}C-CPMAS NMR (100 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in deuterated solvents on a Jeol Resonance ECZ-400R Spectrometer. Quoted chemical shifts are in ppm downfield from tetramethylsilane (TMS) reference using the residual protonated solvents as an internal standard. Ultraviolet- visible (UV-vis) spectra were measured with Agilent Cary 5000 UV-Vis-NIR spectrophotometer. Electrochemical studies were done using Gamry, INTERFACE1010 31184 in three electrode system were Pt wire as a counter electrode, Ag/AgCl as a reference electrode and Glassy carbon as a working electrode. Tetrabutylammonium perchlorate as an electrolyte and HPLC grade dichloromethane as a solvent. Finally, the redox potentials were modified with reference to the ferrocene (Fc/Fc^{+}). The HOMOs are calculated as HOMO =-(4.8+oxd. potential) and LUMO as LUMO=-(4.8+red. potential).

Experimental Section

Synthetic procedure for polymer (**nQ1**):

To a mixture of tris-(4-formylphenyl) amine (1 eq.) and N, N-diacetyl-piperazine- 2,5-dione (1.5 eq.) and K_2CO_3 (4 eq.), DMF (5 mL) was syringe injected under N_2 atmosphere. The reaction mixture was stirred at 100 °C for 4 days. The reaction mixture is cooled to room temperature, poured into ice-cooled water, the precipitate was collected by filtration and washed with DMF, water, methanol. The insoluble solid of diarylidene-diketopiperazine polymer (**nQ1**) was used for the next step after soxhlet extraction with tetrahydrofuran.

Synthetic procedure for *p*-azaquinodimethanes polymer (**Q1**):

A mixture of **nQ1** (1 eq.), K_2CO_3 (5 eq.) and alkyl bromide (4 eq.) in DMF (10 mL) was stirred at room temperature for 2 days under N_2. The reaction mixture was poured into water and filtered the solid and washed with DMF, plenty of water, methanol, and acetone.

Electrochemical measurement

Electrode Fabrication: For electrochemical measurements, glassy carbon electrode was coated with active materials (polymers **nQ1** or **Q1**). The material paste is made in 500 µl NMP, polymer (5 mg), Nafion binder (100 µl), and carbon black (0.66 mg) were added. The solution was stirred for 16 h to make the solution homogeneous. In the next step, 0.1 µl of the solution was drop casted on the glassy carbon electrode. Finally, the electrode was vacuum dried for 1-2 hrs.

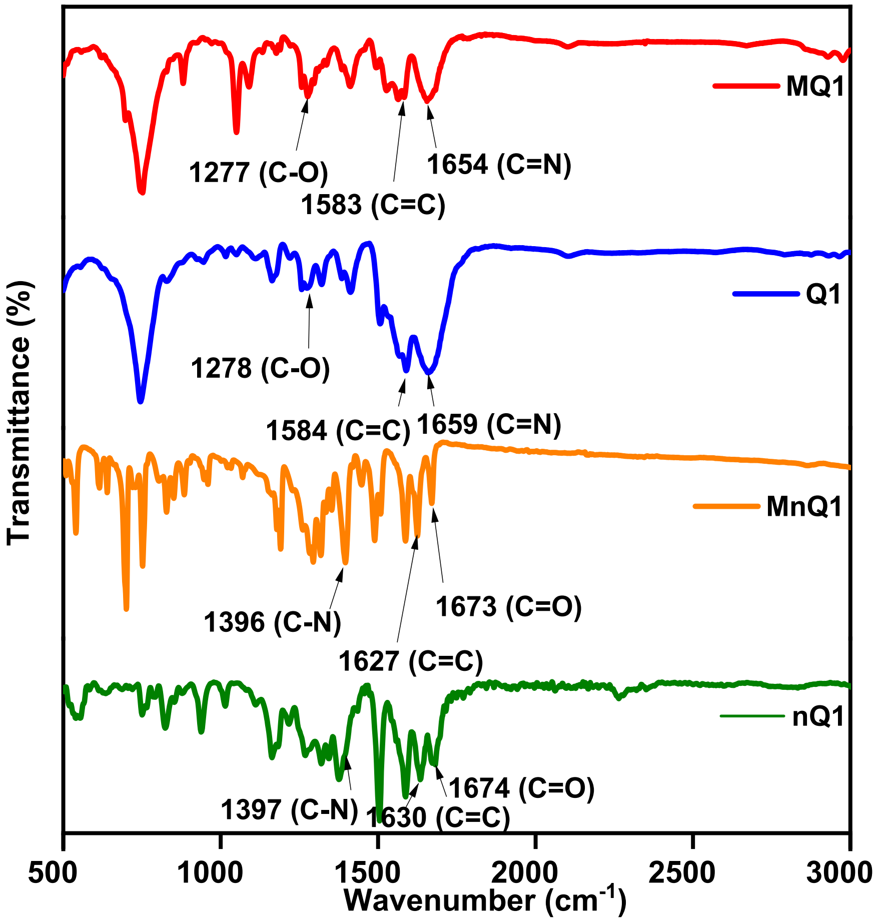


Fig. S1: FT-IR spectra of model compounds **MnQ1**, **MQ1** and polymers **nQ1**, **Q1**

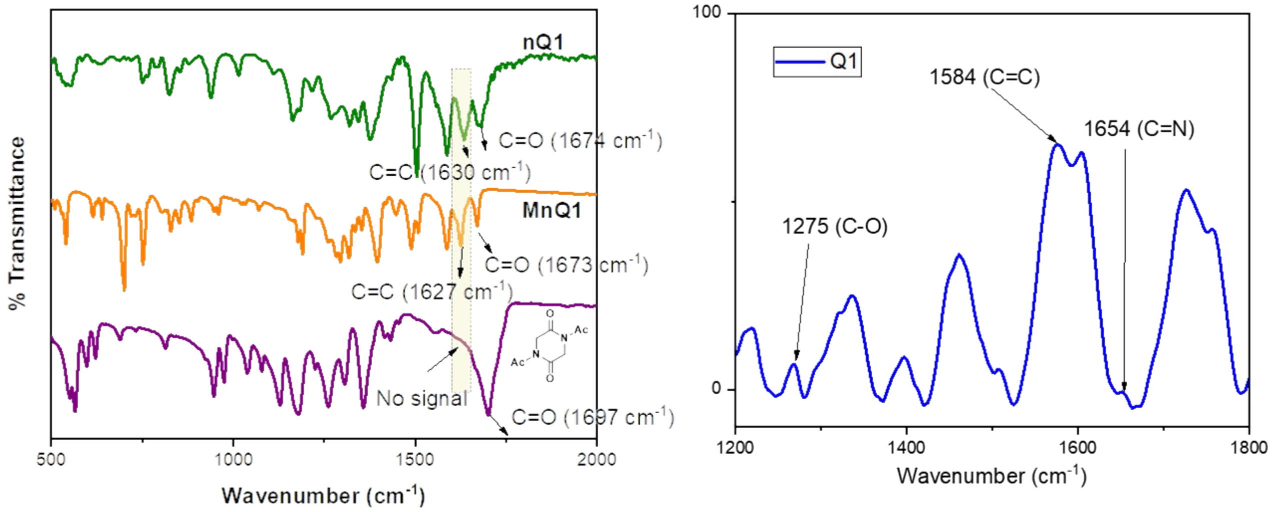


Fig. S2: a) FT-IR spectra of **PA**, **MnQ1** and **nQ1** b) Raman spectra of **Q1**.

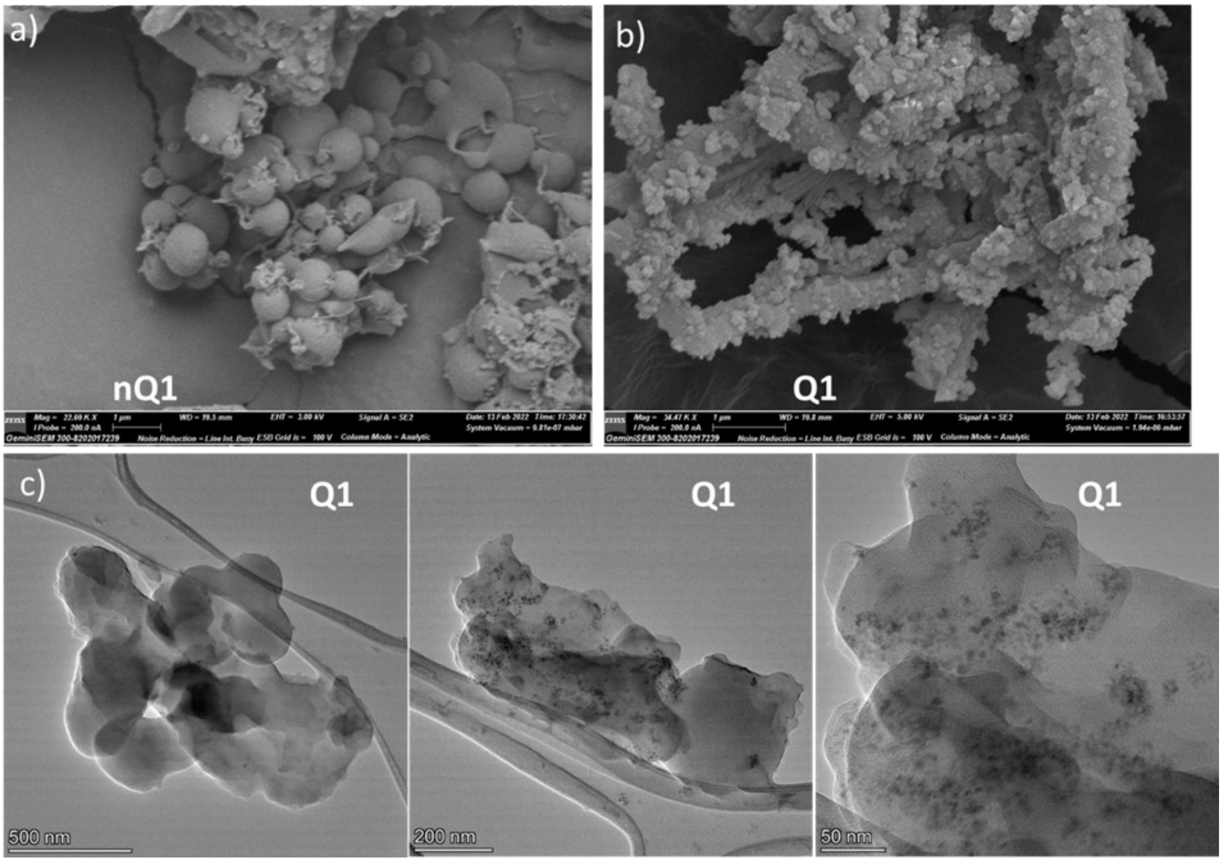
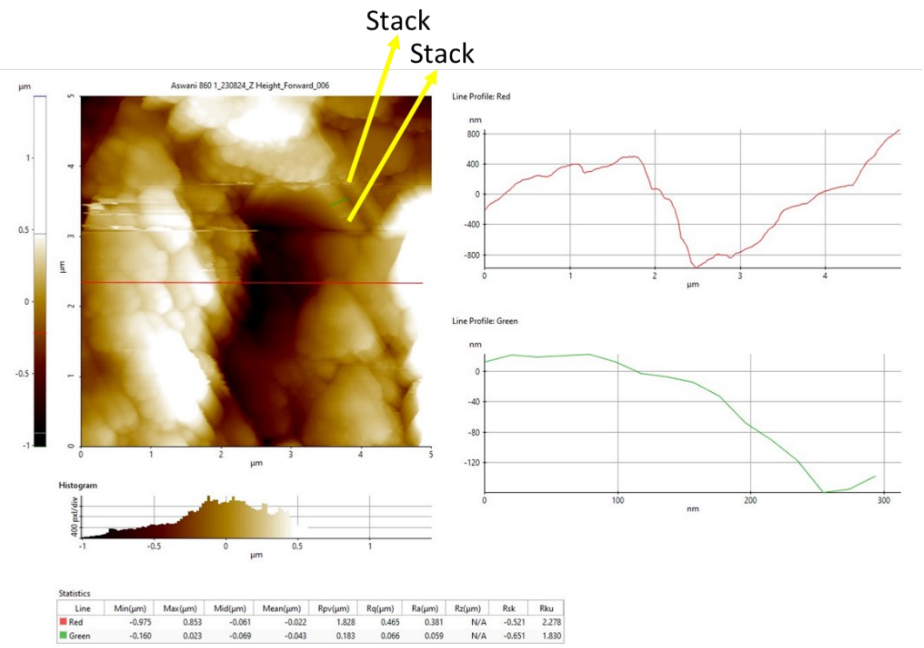


Fig. S3: FE-SEM images of a) **nQ1** and b) **Q1** and c) HR-TEM images of **Q1**.



Statistics

Line	Min(µm)	Max(µm)	Mid(µm)	Mean(µm)	Rpv(µm)	Rq(µm)	Ra(µm)	Rz(µm)	Rsk	Rku
🟥 Red	-0.975	0.853	-0.061	-0.022	1.828	0.465	0.381	N/A	-0.521	2.278
🟩 Green	-0.160	0.023	-0.069	-0.043	0.183	0.066	0.059	N/A	-0.651	1.830

Fig. S4: AFM image of **Q1**

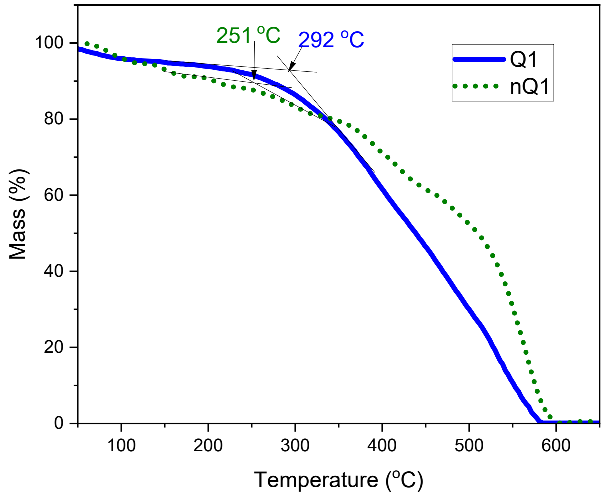


Fig. S5: Thermogravimetric analysis of **nQ1** and **Q1**.

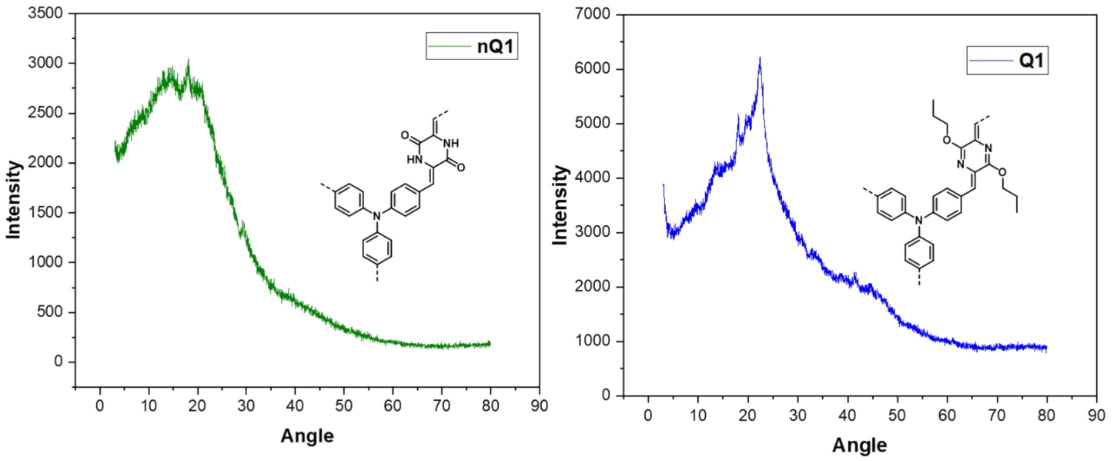


Fig. S6: Powder XRD of a) **nQ1** and b) **Q1**.

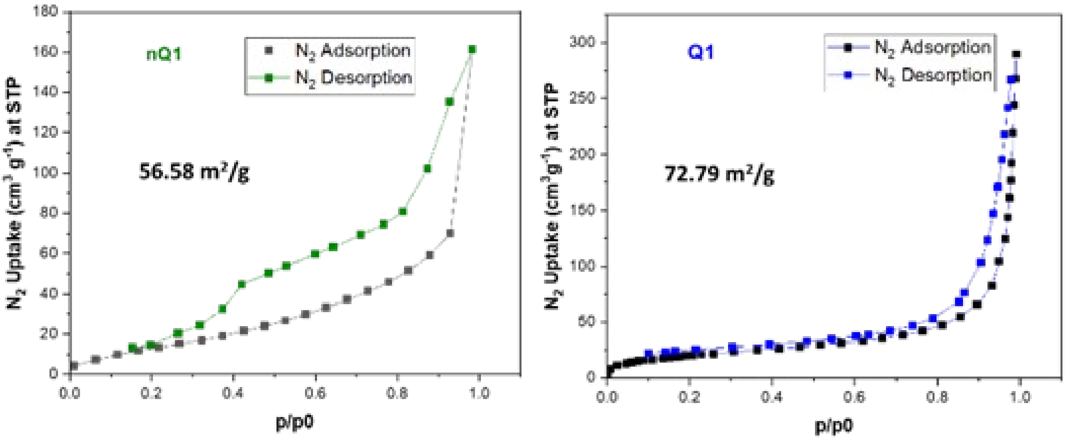


Fig. S7: Nitrogen adsorption and desorption isotherms of a) **nQ1** and b) **Q1**.

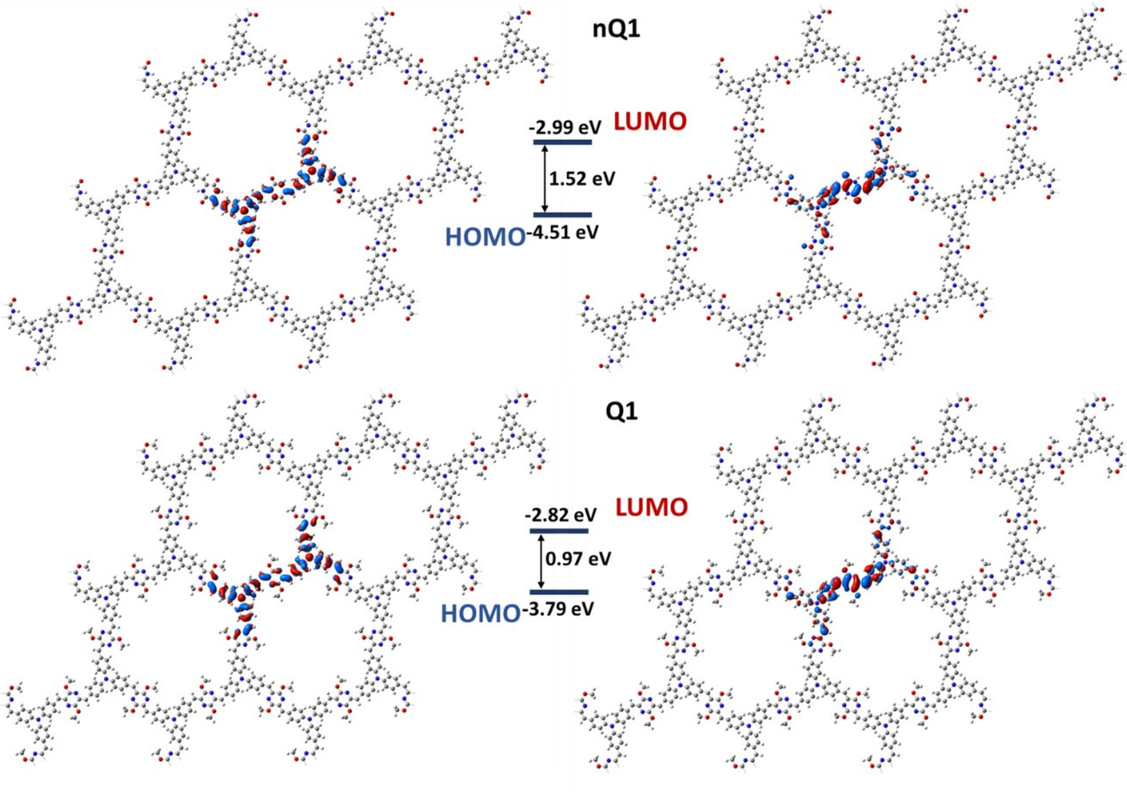


Fig. S8: DFT-optimized HOCO and LUCO of **nQ1** and **Q1**.

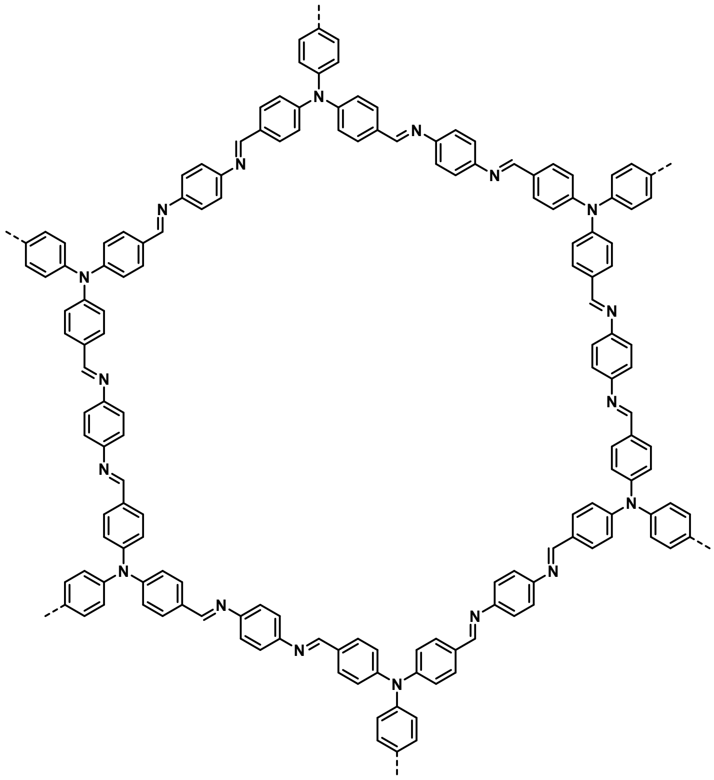


Fig. S9: Imine based polymer (**M1-P**)

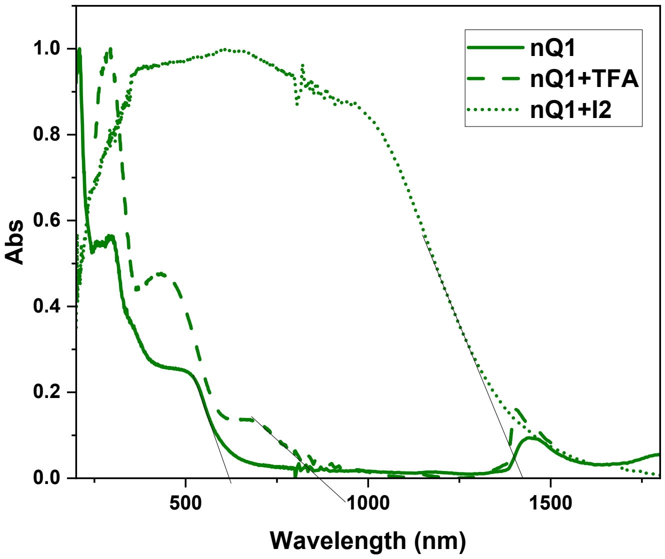


Fig. S10: Comparison of the UV-Vis absorption spectra of **nQ1** with **nQ1** in TFA and iodine.