Phthalocyanine Based Porous Organic Polymer for Lithium Ion Battery Anode

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Experimental details:

(1) Synthesis of 2(3),9(10),16(17),23(24)-tetraiodophthalocyanine $H_2Pc(I)_4$

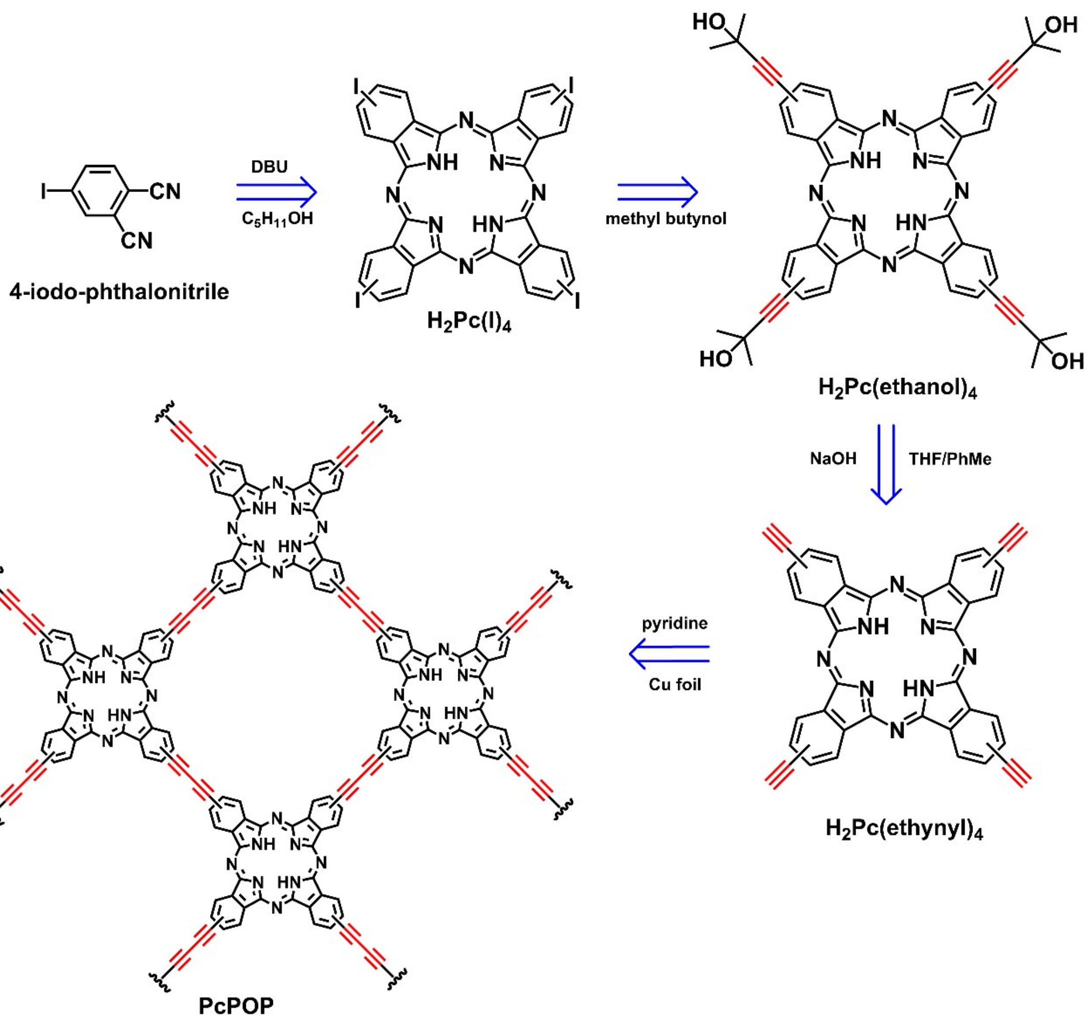
4-iodo-phthalonitrile (1 g) was added into a 25 mL reaction tube with pentanol (8 mL) and DBU (8 drops) under the protection of N_2. The reaction was heated to 110 °C for 4h. After the reaction, the product was purified by silica gel column with CH_2Cl_2/ hexane (V/V, 6/1) as the eluent. Repeated chromatography followed by recrystallization from methanol and dichloromethane gave a purified product $H_2Pc(I)_4$ (480 mg, 48%) as green powder.

(2) Synthesis of 4,4',4'',4'''-(phthalocyanine-2(3),9(10),16(17),23(24)-tetrayl)tetrakis(2-methyl but-3-yn-2-ol) $H_2Pc(ethanol)_4$

β-tetraiodine phthalocyanine (344 mg), bis (triphenylphosphine) palladium dichloride (3.0 mg), and CuI (0.3 mg) were added to a 25 mL reaction tube. Under N_2 protection, THF (4 mL), triethylamine (8 mL), and methyl butynol (732 μL) were added and reacted at room temperature for 24h. The solvent was removed by vacuum distillation, and the sample was purified with THF/hexane (V/V, 6/1). Repeated chromatography followed by recrystallization from THF and hexane gave a purified product $H_2Pc(etynol)_4$ (95 mg, 34%) as green powder.

(3) Synthesis of 2(3),9(10),16(17),23(24)-tetra ethynyl phthalocyanine $H_2Pc(ethynyl)_4$

β-tetraethylenol phthalocyanine (264 mg) and NaOH (148 mg) were added to a 25 mL reaction tube. Under the N_2 protection, THF (6 mL) and toluene (6 mL) were added. Then, the tube was heated to 90°C and reacted for 12h. After the reaction, the solvent was distilled and the product was recrystallized with THF/hexane to obtain $H_2Pc(ethynyl)_4$ (65 mg, 31%) as green powder.



Scheme S1 The synthetic route for PcPOP.

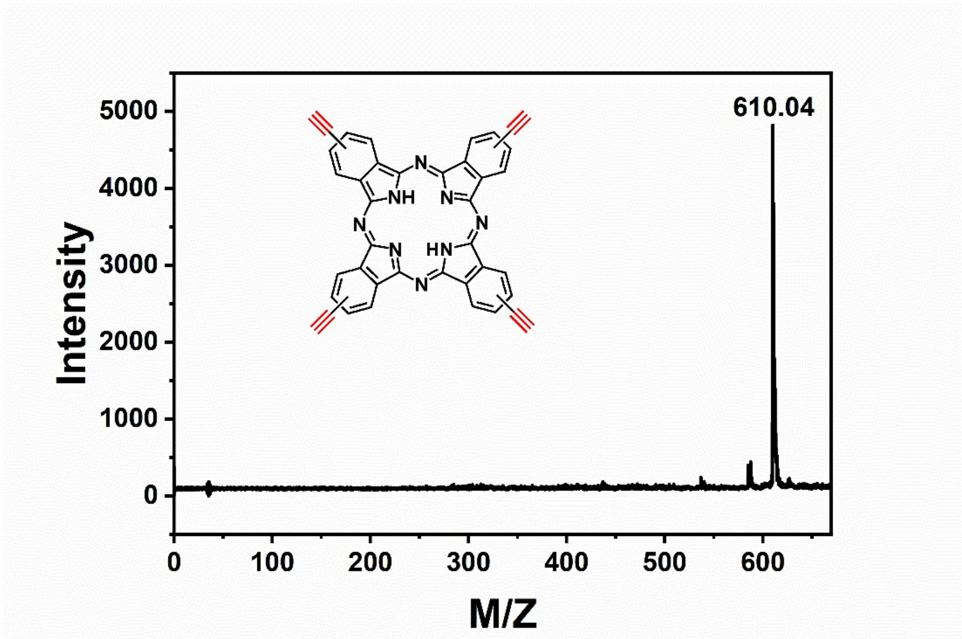


Fig.S1 MS spectrum of 2(3),9(10),16(17),23(24)-tetraethynylphthalocyanine $H_2Pc(ethynyl)_4$.

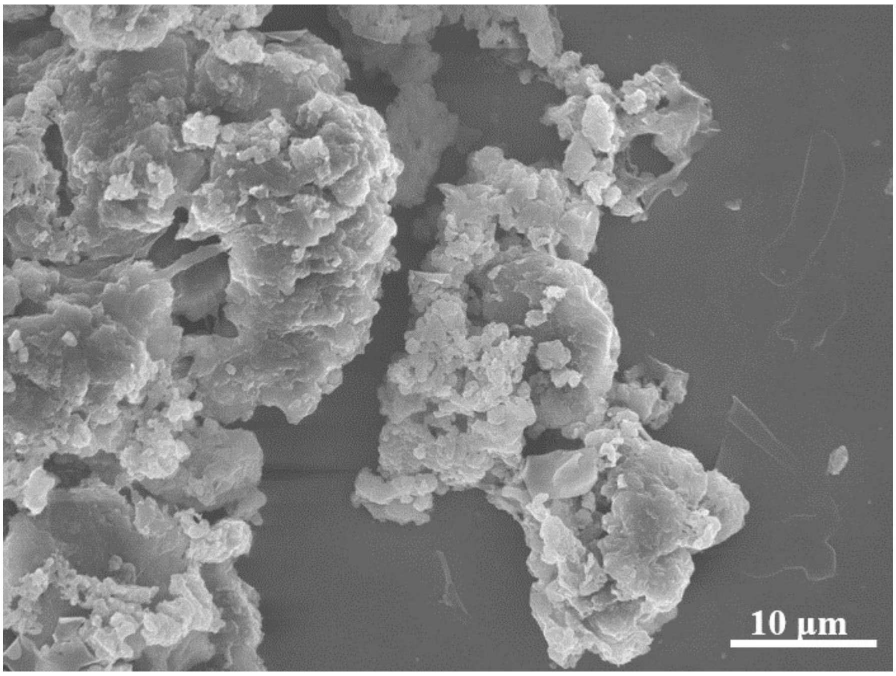


Fig.S2 SEM image of PcPOP (EDS mapping).

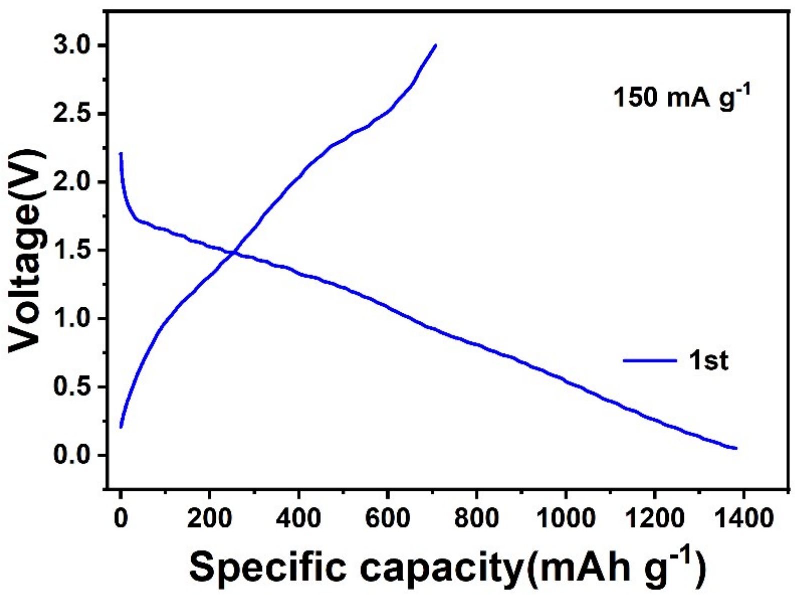


Fig.S3 First charge/discharge curves of the PcPOP under the current density of 150 mA g^{-1}.

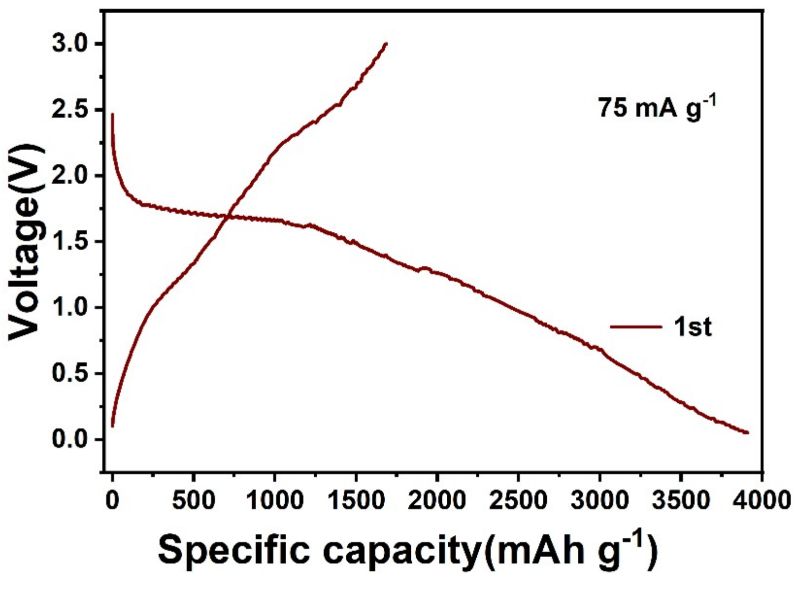


Fig.S4 First charge/discharge curves of the PcPOP under the current density of 75 mA g^{-1}.

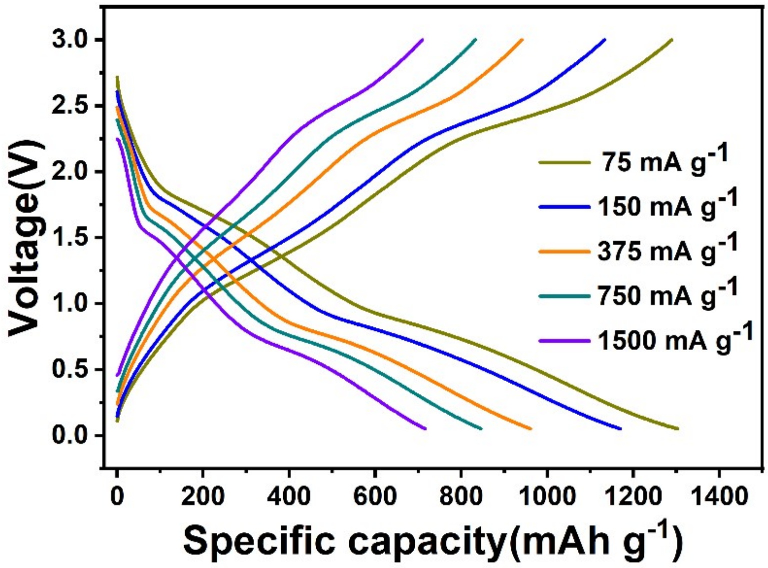


Fig.S5 Charge/discharge curves of the PcPOP at different current densities.

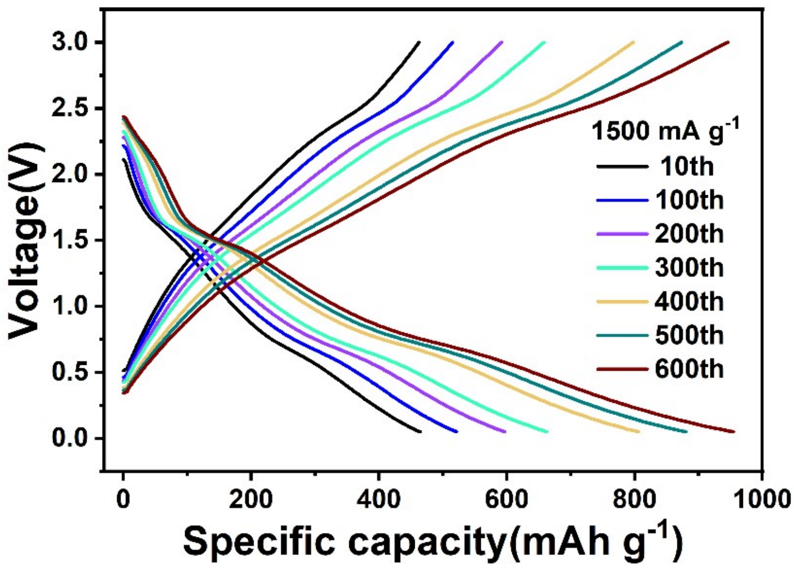


Fig.S6 Charge/discharge curves of PcPOP electrode at the current density of 1500 mA g^{-1}.

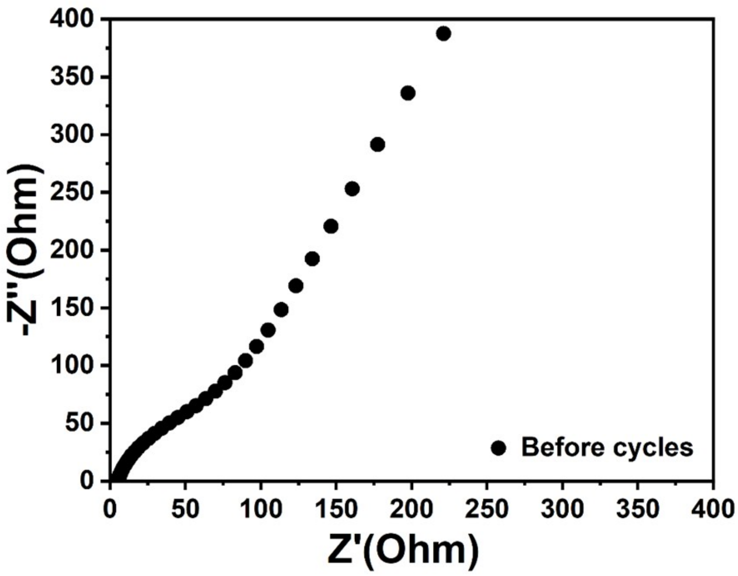


Fig.S7 Nyquist plot of the PcPOP electrodes before cycles.