

Supporting information

Nitrogen doped Small Molecular Structure of Nano-graphene Observed Their Dynamic Hierarchical Self-assemble Properties for High Performance Anodes Lithium Ion Storage

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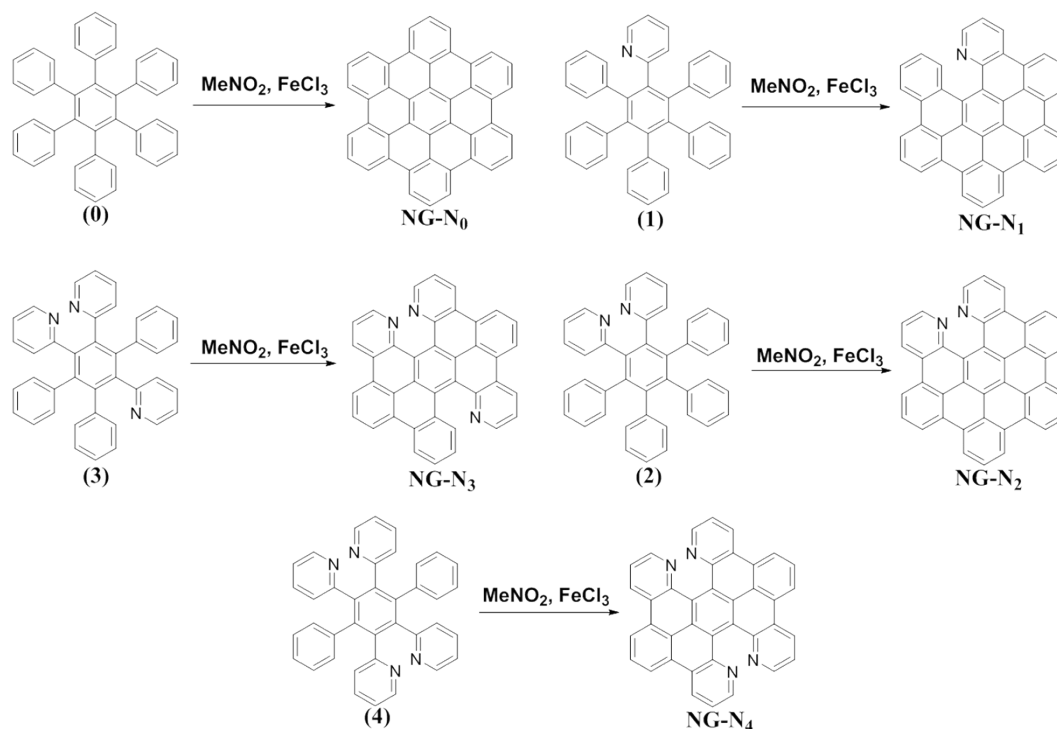
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General Information on Techniques

Mass spectra were measured on a Waters Xevo OTof MS with an ASAP probe. Electrospray ionization (ESI) mass spectra were recorded on a Thermoquest Trace. Elemental analyses were performed using a Carlo Erba Instruments CHNS-O EA1108 analyzer.



Scheme-1. Routes of the N-doped NG-N₀₋₄ derivatives: design and synthesis.

1.1. Materials synthesis

2-(2-Phenylethynyl)pyridine ^[1], 2,2'-(1,2-ethynediyl)bis-pyridine ^[2] 2,3,4,5-tetraphenyl-2,4-Cyclopentadien-1-one ^[3], 2,5-diphenyl-3,4-di-2-pyridinyl-2,4-Cyclopentadien-1-one^[4], 3',4',5',6'-tetraphenyl-1,1':2',1''-Terphenyl^[5], 2-(4',5',6'-triphenyl-[1,1':2',1''-terphenyl]-3'-yl)pyridine^[6], 2,2'-(3',6'-diphenyl-[1,1':2',1''-terphenyl]-4',5'-diyl)dipyridine^[7], 2,2',2''-(5'-phenyl-[1,1':2',1''-terphenyl]-3',4',6'-triy)tripyrindine^[6] and 2',3',5',6'-tetra(pyridin-2-yl)-1,1':4',1''-terphenyl were synthesized according to a previously reported procedure^[9,10]. All other reagents were used as received from commercial sources.

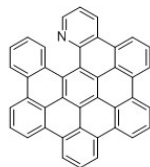
1.2. General Procedure for oxidation cyclization reaction

Compound 2',3',5',6'-tetra(pyridin-2-yl)-1,1':4',1''-terphenyl (0.8g, 1.49mmol) was dissolved in dry dichloromethane (40 mL). The solution was degassed via bubbling nitrogen for 10min. Then FeCl₃ (3.37g, 20mmol) in dry nitromethane (7 mL) was added slowly via a syringe. The resulting mixture was kept under nitrogen flow during the entire reaction. After 3 h, the reaction was quenched with a large volume of methanol. The dark precipitate was collected and washed with methanol / acetone / dichloromethane (1:1:1). The final brown precipitate was then collected and dried in a vacuum to afford NG-N₄ Yield: 0.3 g (37%). ESI-MS (M + H)⁺:530.39 for Calculated 530.59; Found, %: C, 86.06; H, 3.45; N, 10.58. C₃₈H₁₈N₄. Calculated, %: C, 86.02; H, 3.42; N, 10.56.

Synthesis of NG-N₃. A procedure analogous to the preparation of NG-N₄ was used and a reddish brown solid. Yield: 0.19 g (32%). ESI-MS (M + H)⁺: 529.60 for Calculated 529.12; Found, %: C, C, 88.47; H, 3.63; N, 7.92. C₃₉H₁₉N₃. Calculated, %: C, 88.45; H, 3.62; N, 7.93.

Synthesis of NG-N₂. A procedure analogous to the preparation of NG-N₄ was used and a yellowish-brown solid. Yield: 0.14 g (28%). ESI-MS (M + H)⁺: 527.02 for Calculated 526.60; Found, %: C, 91.22; H, 3.42; N, 5.37. C₄₀H₁₈N₂. Calculated, %: C, 91.23; H, 3.45; N, 5.32.

Synthesis of NG-N₁. A procedure analogous to the preparation of NG-N₄ was used and a yellowish solid. Yield: 0.15 g (34%). ESI-MS (M + H)⁺: 525.34 for Calculated 525.61; Found, %: C, 93.68; H, 3.66; N, 2.67. C₄₁H₁₉N. Calculated, %: C, 93.69; H, 3.64; N, 2.66.



Chemical Formula: C₄₁H₁₉N
Molecular Weight: 525.61

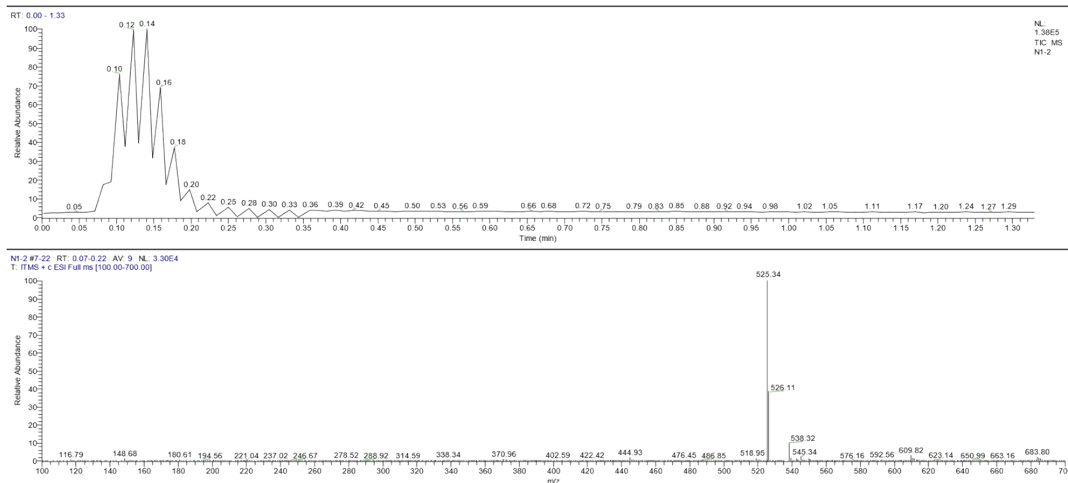
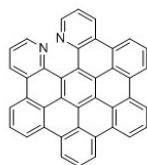


Figure S1. ESI-MS spectrum of NG-N1



Chemical Formula: C₄₀H₁₈N₂
Molecular Weight: 526.60

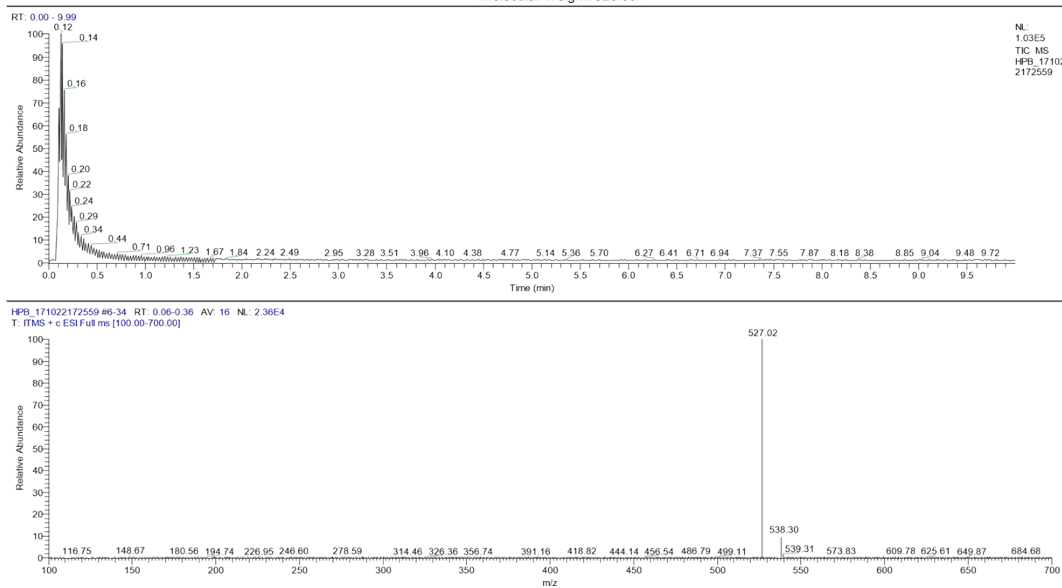
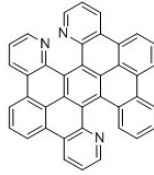


Figure S2. ESI-MS spectrum of NG-N2



Chemical Formula: $C_{38}H_{19}N_3$
Molecular Weight: 529.60

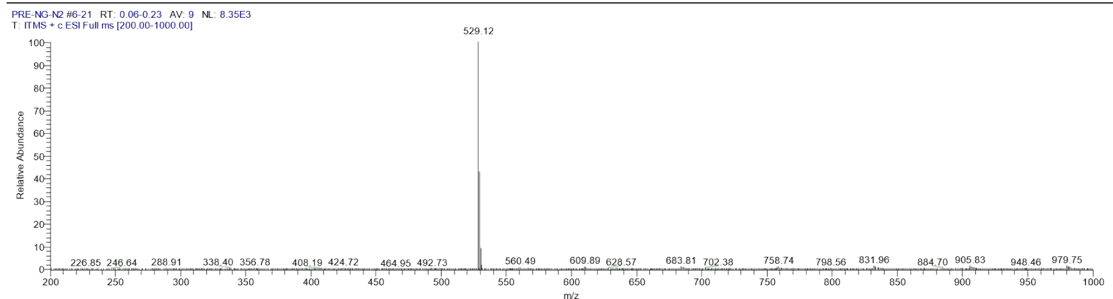
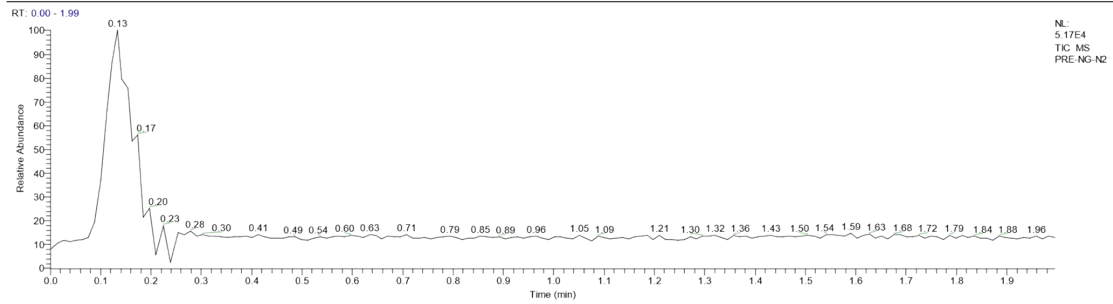
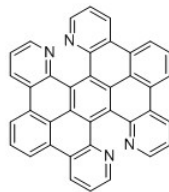


Figure S3. ESI-MS spectrum of NG-N3



Chemical Formula: $C_{38}H_{18}N_4$
Molecular Weight: 530.59

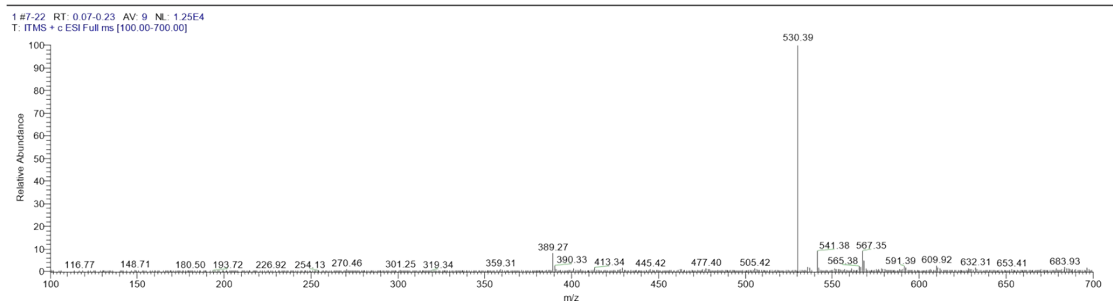
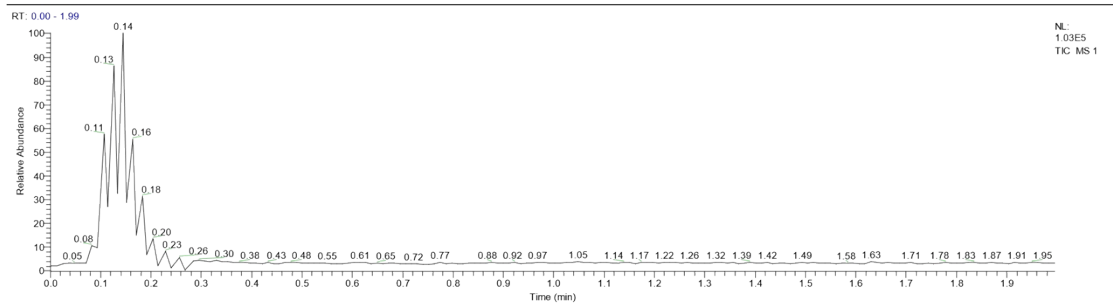


Figure S4. ESI-MS spectrum of NG-N4

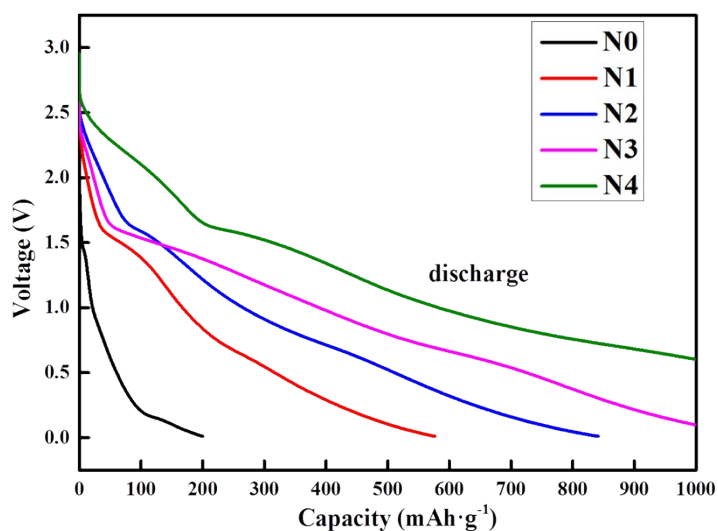


Figure S5. The galvanostatic discharge voltage profiles of NG-N_{0.4} anode.

References

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