

Supporting Information

Bacterial Cellulose-Polyaniline Composite derived Hierarchical Nitrogen-Doped Porous Carbon Nanofibers as Anode for High Rate Lithium-Ion Batteries

Mani Pujitha Illa^{1,2}, Anil D Pathak², Chandra S. Sharma², Mudrika Khandelwal^{1,}*

¹Department of Materials Science and Metallurgical Engineering,

Indian Institute of Technology, Hyderabad, Kandi-502285, Sangareddy, Telangana, India

²Creative & Advanced Research Based on Nanomaterials (CARBON) Laboratory,

Department of Chemical Engineering,

Indian Institute of Technology, Hyderabad, Kandi-502285, Sangareddy, Telangana, India.

*Corresponding author email: mudrika@msme.iith.ac.in

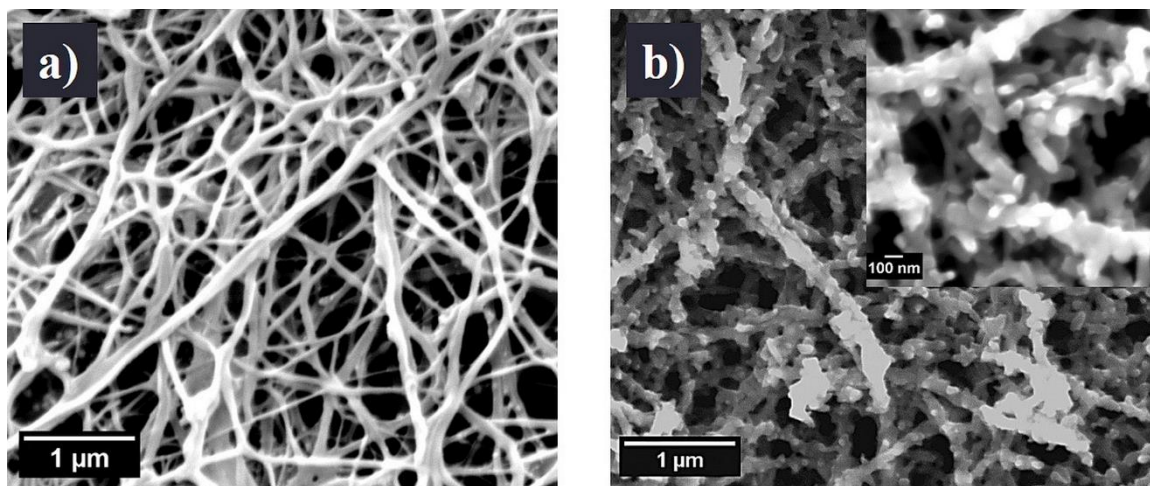


Figure S1. a) SEM micrograph of BC b) SEM micrograph of carbonized BC-PANI

Table S1 Textural properties of BC-PANI composite and its derived carbon

Sample	Type of isotherm	Specific surface area [m^2g^{-1}]	Micro pore area [m^2g^{-1}]	Average Pore volume [ccg^{-1}]
BC-PANI	II	25	-	0.12
Carbonized BC-PANI	II	159	109	0.25
BC-PANI_AC	IV	2037	1004	0.75

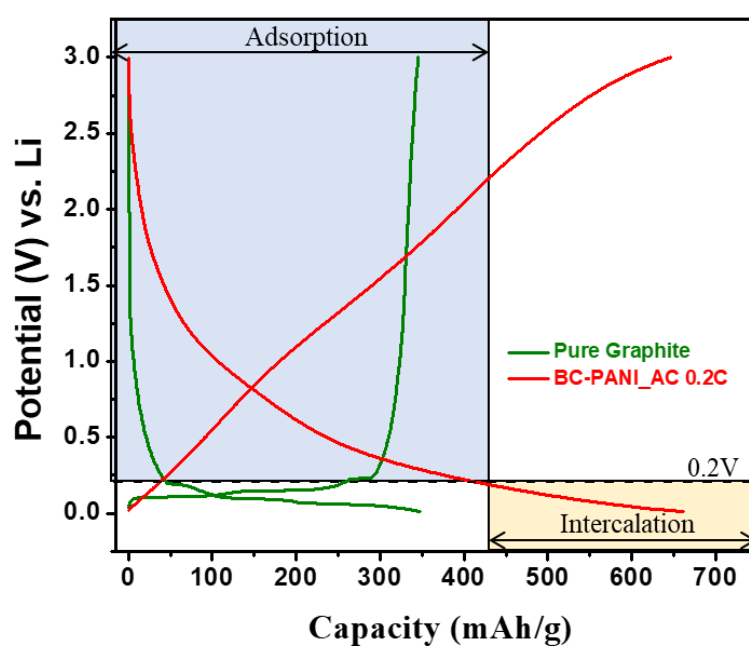


Figure S2. Charge-discharge curves of BC-PANI_AC and pure graphite at 0.2C

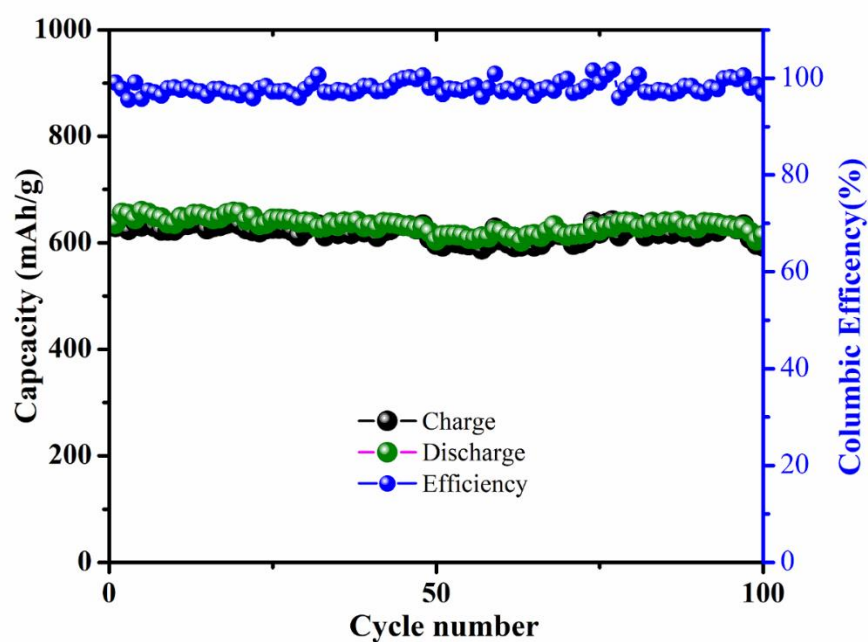


Figure S3. Cyclic stability performed at 0.2C

Table S2. Calculation of % interaction of nitrogen structures with lithium

Structure	Calculated binding energy (KJ/mol)	Normalised B.E	Atomic Contribution (%) based on area under curve from XPS	Relative contribution (From binding energy and atomic%)
	(A)	$(B_i = A_i / \sum A \times 100)$	(C _i)	$(D = 100 \times (B_i \times C_i) / \sum BC)$
Pyrrolic N	-578	30	66	63
Pyridine N	-735	38	10	12
Oxidized N	-604	32	24	25
Total	-1917	100	100	100

Calculation example for Pyrrolic N:

The calculated binding energy (B.E) of Li for Pyrrolic N from DFT = -578 KJ/mol.

$$\text{Therefore, Normalised B. E} = \frac{B.E \text{ of Pyrrolic N}}{B.E.of \text{ pyrrolic N} + B.E.of \text{ pyridine N} + B.E.of \text{ oxidized N}}$$

$$= \frac{-578}{-1917}$$

$$= \sim 30\%$$

The atomic contribution (%) of Pyrrolic N based on area under curve from XPS = 66%

$$\text{Relative contribuion of pyrrolic N (From B. E and XPS atomic \%)} = \frac{30 \times 66}{30 \times 66 + 38 \times 10 + 32 \times 24}$$

$$= \sim \mathbf{63\%}$$