

Supplementary information

**Defect-Rich Boron doped Carbon Nanotube as  
Electrocatalyst for Hybrid Li-air Battery**

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## Catalogue:

1. Experimental preparation
2. Calculation of DFT
3. Analysis of experimental results

### 1. Experimental preparation

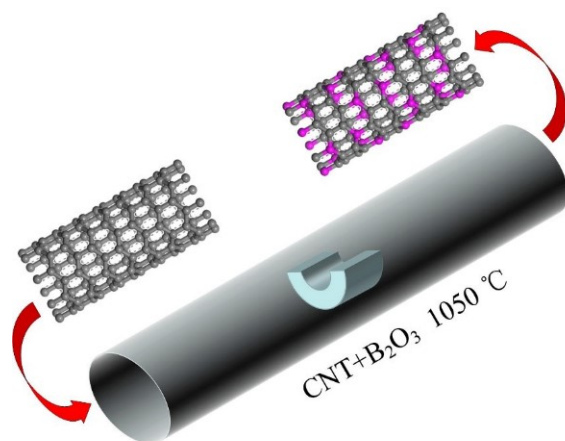


Fig.S1 Schematic illustration of synthesis process of BC<sub>3</sub>NT.

Table S1 List of chemicals

Name	Purity	Manufacturer
LiOH	95%	Sinopharm Group
CNT	99.9%	Beijing Deke Daojin Science and Technology Co., LTD
PTFE		Sinopharm Group
NMP	AR	Sinopharm Group
B <sub>2</sub> O <sub>3</sub>	99%	Sinopharm Group
LISICON		Shenzhen Kejing Star Technology Co.
LITFSI-TEGDME		NJ Scientific.

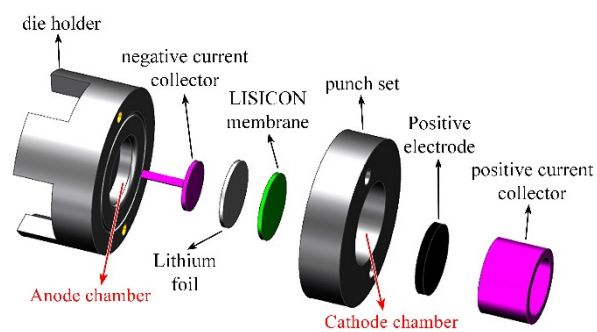


Fig. S2 Illustrate of HLAB mold.

## 2. Calculation of DFT

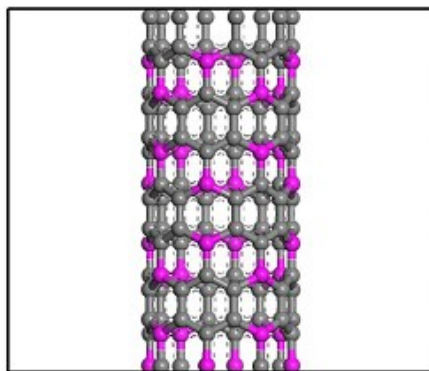


Fig. S3 Model of nanotube.

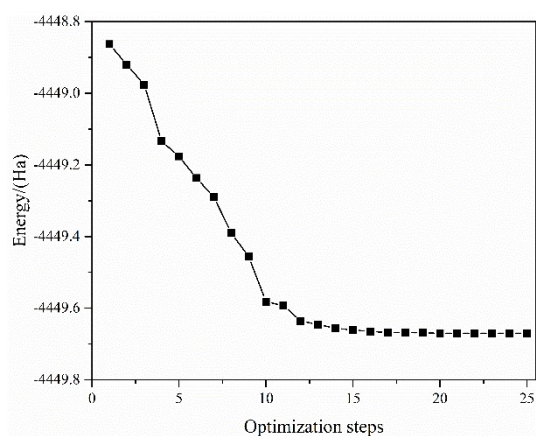
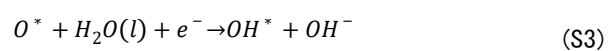
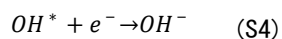


Fig. S4 Energy convergence diagram of optimization process.

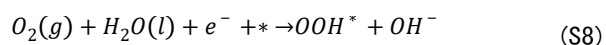
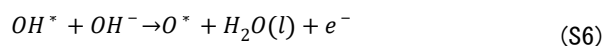
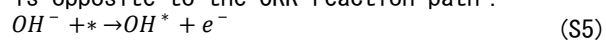
Under alkaline conditions, the ORR and OER four-electron reaction path is in the ESI. †

$$O_2(g) + H_2O(l) + e^- + * \rightarrow OO H^* + OH^- \quad (S1)$$




\* represents the active site on the catalyst surface, and (l) and (g) represent the liquid and gas phases, respectively.

The OER reaction path is opposite to the ORR reaction path :



### 3. Analysis of experimental results

Table S2 Content of element

	B <sub>2</sub> O <sub>3</sub> : CNT=2:1	B <sub>2</sub> O <sub>3</sub> : CNT=5:1	B <sub>2</sub> O <sub>3</sub> : CNT=8:1
C	92.20%	87.86%	88.58%
B	2.84%	4.68%	5.15%
O	4.10%	5.83%	2.98%

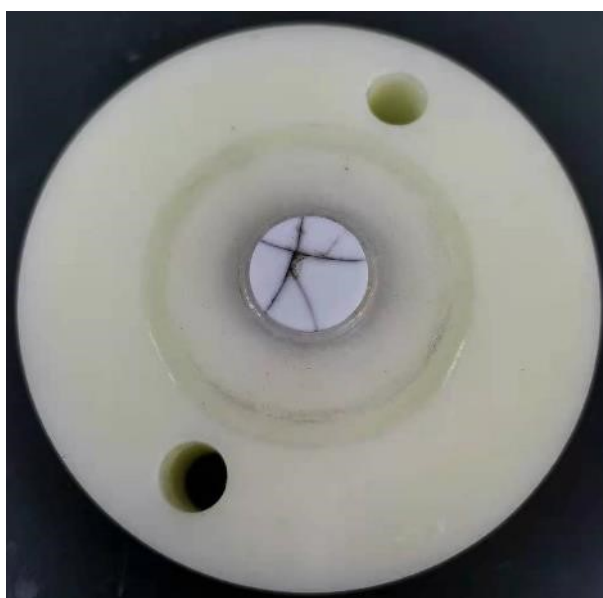


Fig. S5 LISICON membrane after test.

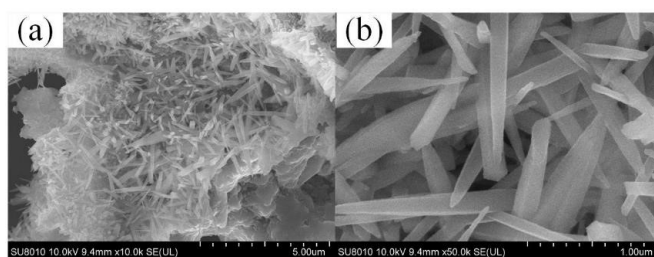


Fig. S6 Lithium dendrites.

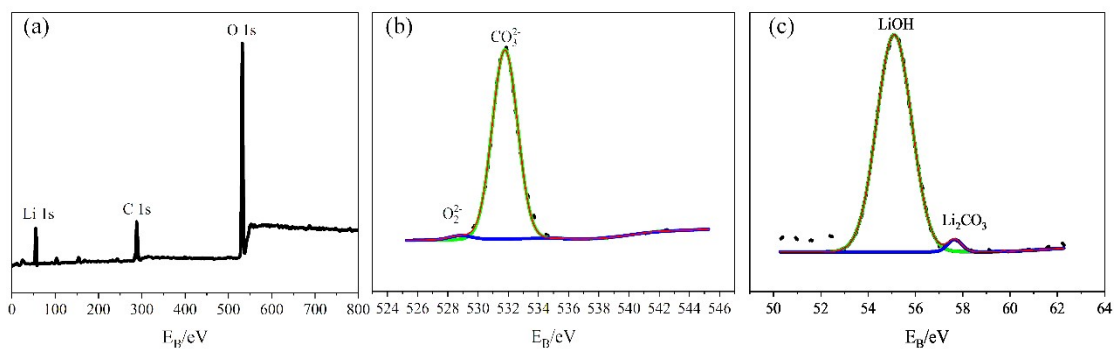


Fig. S7 XPS spectrum: (a) Total, (b) O 1s, (c) Li 1s.

Table S3 Comparison of battery performance

Catalyst	Cycling number	Initial discharge capacity (mAh·g <sup>-1</sup> )	Overpotential (V)	Ref
Boron doped CNT	165	8900	0.3	This work
Pt-carbon paper	50		0.75	Sun <sup>1</sup>
MNO-CNT-CNFFs	21		0.15 (low current)	Ji <sup>2</sup>
Mn <sub>3</sub> O <sub>4</sub>	20	221 (0.5 mA·cm <sup>-2</sup> )	1.3	Li <sup>3</sup>
Graphite			0.47	Zhou <sup>4</sup>

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- (2) Ji, D.; Peng, S.; Safanama, D.; Yu, H.; Li, L.; Yang, G.; Qin, X.; Madhavi, S.; Adams, S.; Ramakrishna, S. Design 3D Hierarchical Architectures of Carbon and Highly Active Transition-Metals (Fe, Co, Ni) as Bifunctional Oxygen Catalysts for Hybrid Lithium-Air Batteries. *Chemistry of Materials* **2017**, *29*. <https://doi.org/10.1021/acs.chemmater.6b05056>.
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