Supporting Information

Synergistic Nitrogen-Doping and Carbon-Coating in N-$MoSe_2$/C Nanoflowers Enable Ultra-high Discharge Capacity for Li-CO_2 Batteries

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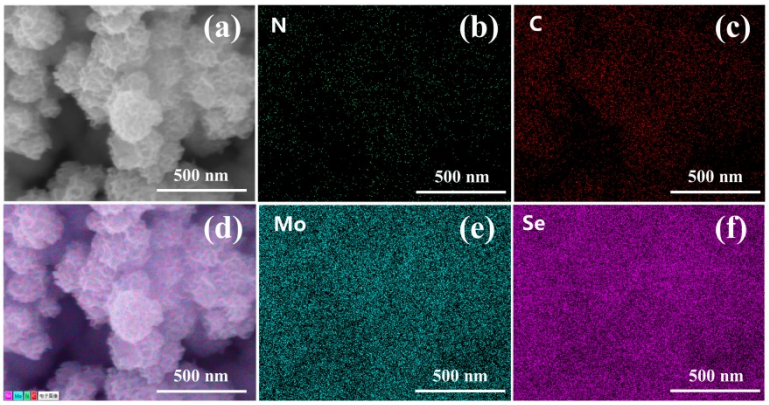

Fig. S1 EDS mapping images of N-$MoSe_2$/C showing the elemental distributions of Mo, Se, N and C.

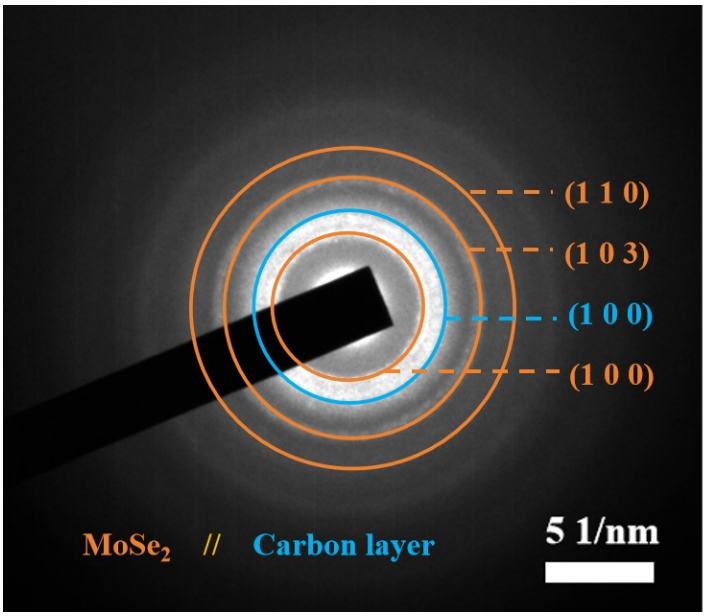

Fig. S2 SAED patterns of $MoSe_2$ and Carbon layer

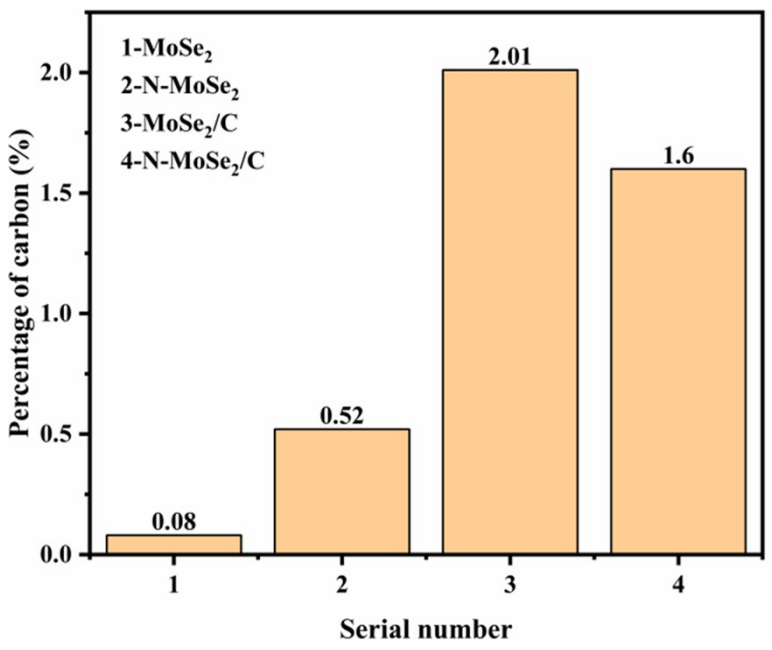

Fig. S3 Carbon content of prepared samples.

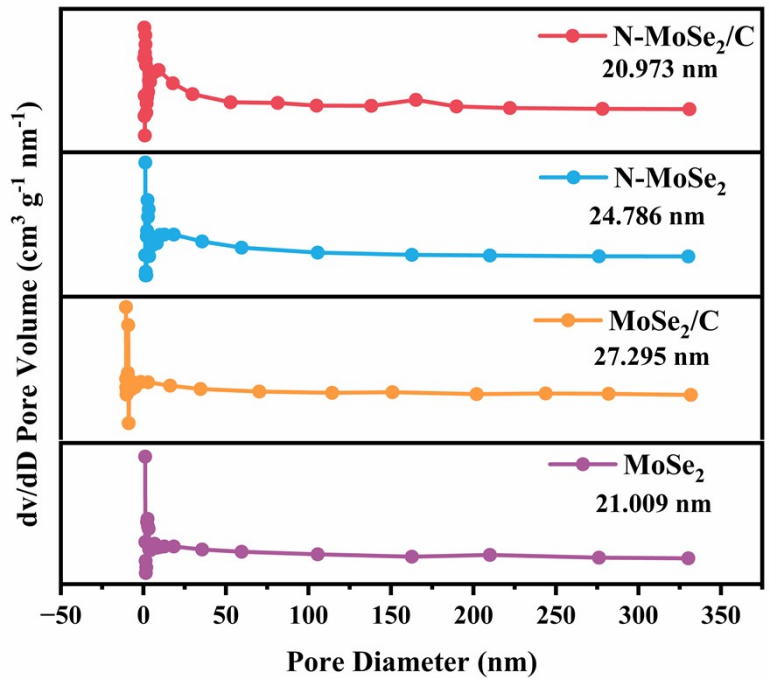

Fig. S4 Pore size testing of corresponding prepared samples.

Table S1. Performance comparison of typical reported cathode catalysts for Li-CO_2 batteries.

Cathode catalyst	Current density (mA g^{-1})	Capacity (mAh g^{-1})	Over potential (V)	Current density (mA g^{-1})	Cut off capacity (mAh g^{-1})	Cycling stability	Ref.
Ru-O-Zr/Ce	100	21075	1.03	100	1000	167	1
MnO_X-CeO_2	100	13631	1.49	100	1000	253	2
CCGA	100	7860	1.53	100	1000	100	3
Cu-Co_4N@CC	100	31000	1.32	200	500	131	4
Ir-Te	100	13247	1.48	1000	1000	350	5
IrRu/N-CNTs	100	6228	<1.5	100	500	>600	6
RuCo NSs/CNT	100	8057	0.94	100	1000	44	7
PdCu/N-CNF	100	18500	1.17	100	1000	270	8
FeCoNiMnCuAl@C	100	27664	1.03	100	1000	134	9
Ru/NS-G	100	12,448	1.4	100	1000	>100	10
MoS_2/CNT	100	8551	1.24	100	500	142	11
Mo_3P/Mo	50	10577	0.13	250	500	78	12
MWCNT/Ru	150	6531	1.30	50	500	50	13
MWCNT/RuNi	200	15165	1.13	200	500	>80	14
N-$MoSe_2$/C	100	37720	1.54	100	500	89	This work

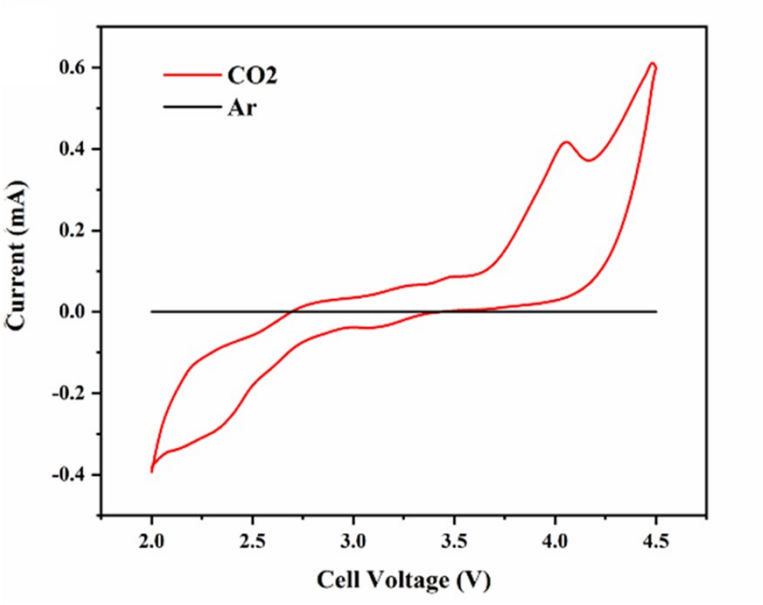

Fig. S5 The discharge performance of N-$MoSe_2$/C at different atmosphere.

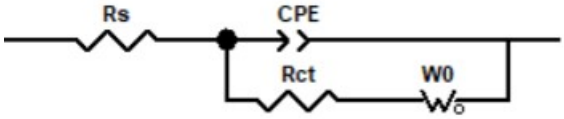

Fig. S6 Equivalent Circuit Model. Rs: Solution Resistance. Rct: Charge Transfer Resistance. CPE: Constant Phase Element. W0: Warburg Resistance

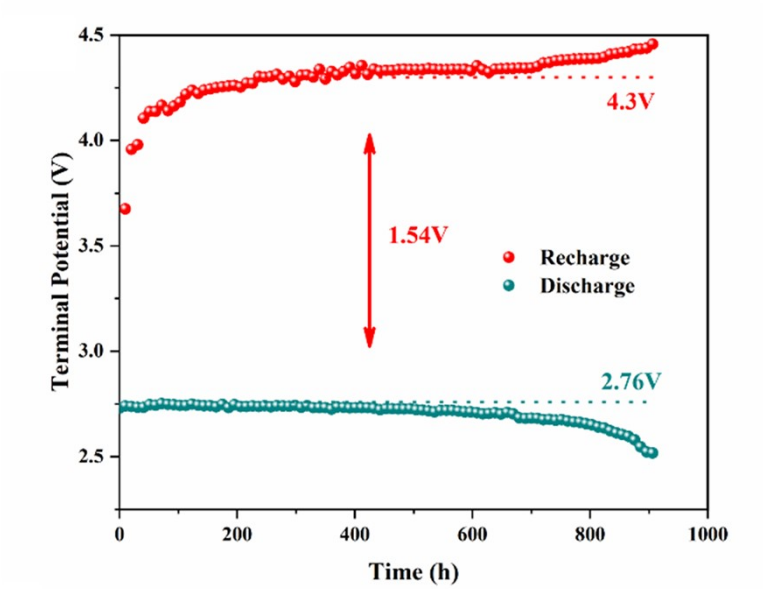

Fig. S7 The cycle performance of N-$MoSe_2$/C assembled battery under the condition of 100 mA g^{-1} current density and cut-off capacity of 500 mAh g^{-1} test.

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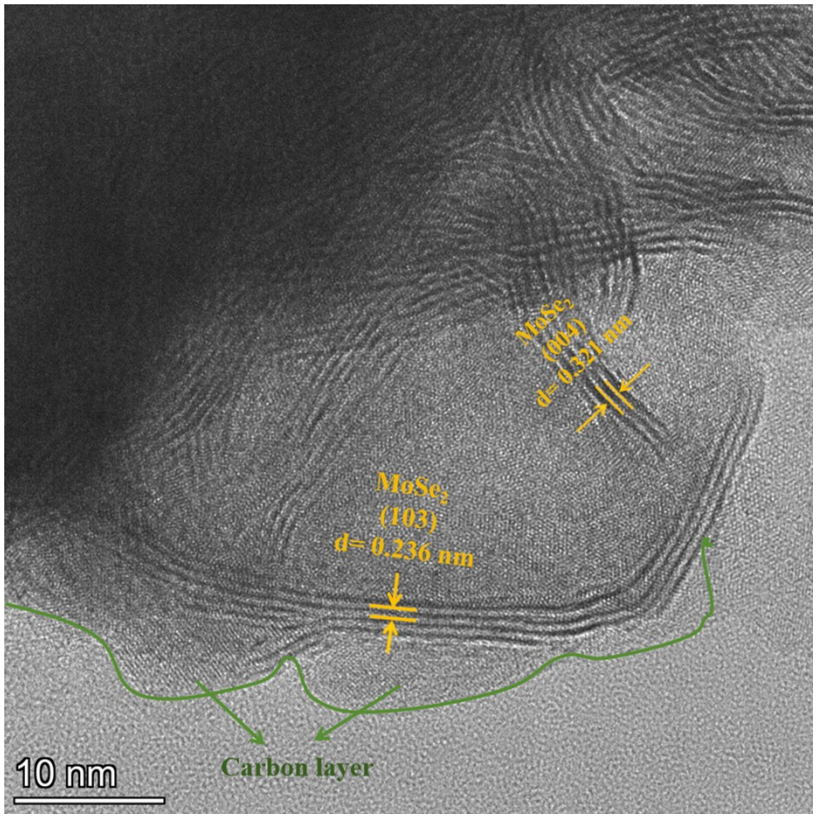

Fig. S8 HRTEM image of N-$MoSe_2$/C nanoflowers after cycling.

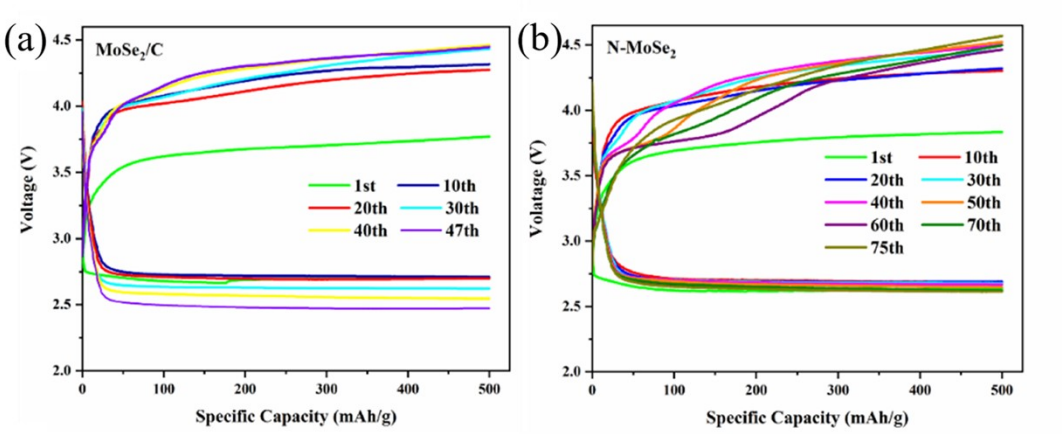

Fig. S9 The cycle stability of (a) $MoSe_2$/C, (b) N-$MoSe_2$ positive electrode under the condition of 100 mA g^{-1} current density and cutoff capacity of 500 mAh g^{-1}

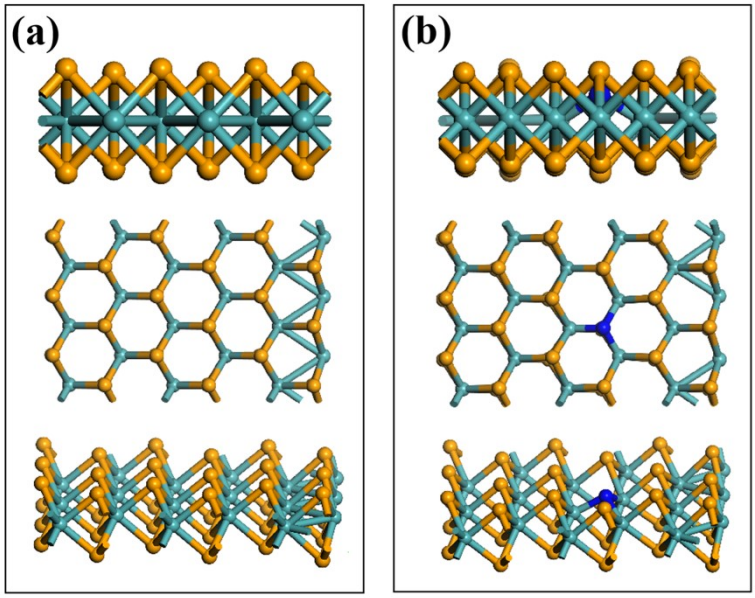

Fig. S10 Optimized structural models: (a) $MoSe_2$(1 0 0) and (b) N-$MoSe_2$(1 0 0).

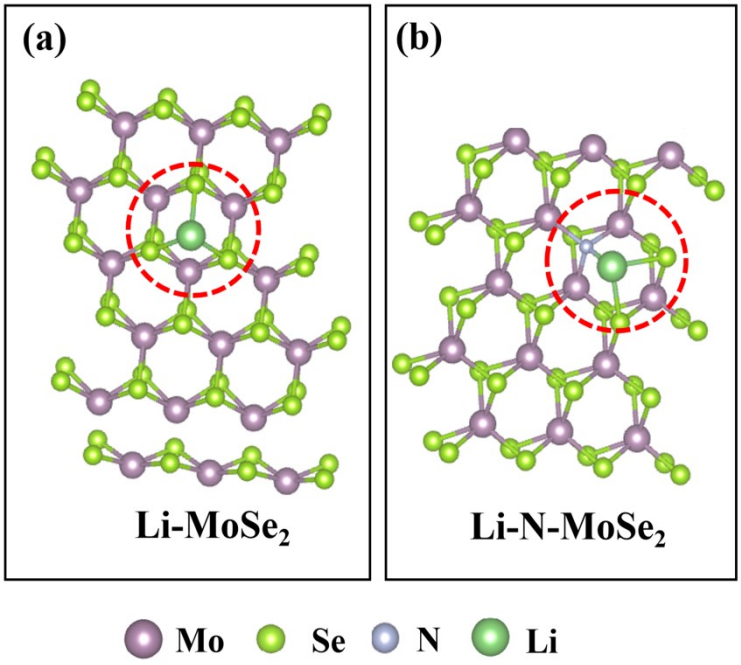

Fig. S11 Structure models of Li with (a) $MoSe_2$ and (b) N-$MoSe_2$.

Supporting Reference

1. Q. Deng, Y. Yang, K. Yin, J. Yi, Y. Zhou, Y. Zhang, *Adv. Energy Mater.*, 2023, **13**, 2302398.
2. Q. Deng, Y. Yang, C. Mao, T. Wang, Z. Fang, W. Yan, K. Yin, Y. Zhang, *Adv. Energy Mater.*, 2022, **12**, 2103667.
3. Q. Deng, Y. Yang, S. Qu, W. Wang, Y. Zhang, X. Ma, W. Yan, Y. Zhang, *Energy Storage Materials*, 2021, **42**, 484-492.
4. X. Ma, W. Zhao, Q. Deng, X. Fu, L. Wu, W. Yan, Y. Yang, *Journal of Power Sources*, 2022, **535**, 231446.
5. Y. Zhai, H. Tong, J. Deng, G. Li, Y. Hou, R. Zhang, J. Wang, Y. Lu, K. Liang, P. Chen, F. Dang, B. Kong, *Energy Stor. Mater.,* 2021, **43**, 391-401.
6. Z. Wang, B. Liu, X. Yang, C. Zhao, P. Dong, X. Li, Y. Zhang, K. Doyle-Davis, X. Zeng, Y. Zhang, X. Sun, *Adv. Funct. Mater.,* 2023, **33**, 2213931.
7. Y. Wang, J. Zhou, C. Lin, B. Chen, Z. Guan, A. M. Ebrahim, G. Qian, C. Ye, L. Chen, Y. Ge, Q. Yun, X. Wang, X. Zhou, G. Wang, K. Li, P. Lu, Y. Ma, Y. Xiong, T. Wang, L. Zheng, S. Chu, Y. Chen, B. Wang, C.-S. Lee, Y. Liu, Q. Zhang, Z. Fan, *Adv. Funct. Mater.,* 2022, **32**, 2202737.
8. P.-F. Zhang, T. Sheng, Y. Zhou, Y.-J. Wu, C.-C. Xiang, J.-X. Lin, Y.-Y. Li, J.-T. Li, L. Huang, S.-G. Sun, Chem. Eng. J. 2022, **448**, 137541.
9. J. Yi, Q. Deng, H. Cheng, D. Zhu, K. Zhang, Y. Yang, *Small*, 2024, **20**, 2401146.
10. Y. Qiao, J. Wu, J. Zhao, Q. Li, P. Zhang, C. Hao, X. Liu, S. Yang, Y. Liu, *Energy Storage Mater.,*2020, **27**, 133-139.
11. C.-J. Chen, C.-S. Huang, Y.-C. Huang, F.-M. Wang, X.-C. Wang, C.-C. Wu, W.-S. Chang, C.-L. Dong, L.-C. Yin, R.-S. Liu, *ACS Appl. Mater. Interfaces,* 2021, **13**, 6156-6167.
12. D. Na, R. K. Kampara, D. Yu, B. Yoon, S. W. Martin, I. Seo, *Mater. Today Energy.* 2023, **38**, 101418.
13. C. Wu, G. Qi, J. Zhang, J. Cheng, B. Wang, *Small*. 2023, **19**, 2302078.
14. K. M. Naik, A. K. Chourasia, M. Shavez, C. S. Sharma, *ChemSusChem*. 2023, **16**,

e202300734.