Supporting Information

Crystalline coordination polymers derived MoS₂ quantum dot doped carbon nanoflakes with ultrafast Li⁺ transfer

Lianshan Sun,*a Chunli Wang, *b,c Huaming Li,a and Limin Wang*b

^a Institute for Energy Research, Key Laboratory of Zhenjiang, Jiangsu University,

Zhenjiang 212013, China

^b State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, CAS, Changchun, 130022, China.

^c International Collaborative Laboratory of 2D Materials for Optoelectronics Science and Technology of Ministry of Education, Institute of Microscale Optoelectronics, Shenzhen University, Shenzhen, 518060, China.

*E-mail: <u>lssun@ujs.edu.cn;</u> <u>clwang@ciac.ac.cn;</u> <u>lmwang@ciac.ac.cn</u>

Materials

All the reagents were used without further purification.

Dopamine hydrochloride (DA-HCl, 98%), sodium molybdate dehydrate (Na₂MoO₄·2H₂O), sodium lauryl sulfate, sulfur powder were from Sigma-Aldrich. MoS₂ quantum dot was from Xianfeng nano Materials Technology Co. Ltd.

Synthesis of MoS₂-N-C nanoflakes

In a typical process, 0.1 g sodium molybdate dihydrate was dissolved in 300 ml of deionized water with stirring, then 0.3 g sodium lauryl sulfate was dissolved in the solution with ultrasonic. Then, 0.1 g dopamine hydrochloride was added in the above solution with vigorous stirring. After stirring for 12 h, the generated 2D precursors were collected by suction filtration and washed with deionized water and ethanol for three times by centrifugal separation, then dried in air dry oven under 70 °C. Then the as-synthesized 2D precursor were mixed with excess sulfur powder by grinding and annealed under Ar flow atmosphere at 700 °C for 2 h, with a heating rate of 5 °C min⁻¹.

Synthesis of N-C nanoflakes

N-C nanoflakes was prepared by NaCl template method. In a typical synthesis, 100 mg dopamine hydrochloride was dissolved in 10 ml deionized water, then mixed well with 100 g NaCl, then the mixture was refrigerated at a low temperature for 24 h. Then the frozen mixture is freeze-dried for 2 days. Then the dried mixture was annealed under Ar flow atmosphere at 700 °C for 2 h, with a heating rate of 5 °C min⁻¹.

Then then products was wash with deionized water to remove NaCl template, then dried at 70 °C for use.

Materials characterization

Morphologies and structures of the products were characterized with scanning electron microscopy (SEM, Hitachi S-4800 field emission scanning electron microscope at an accelerating voltage of 10 kV and 15 kV) and transmission electron microscopy (TEM, FEI Tecnai G2 S-Twin instrument). The N₂ adsorption–desorption isotherm was performed on a Micromeritics ASAP 2020 instrument. The crystallographic information was collected by a powder X-ray diffraction (XRD, Bruker D8 Focus and D/max 2500pc power X-ray diffractometer using Cu Kα radiation at a scan rate of 5° min⁻¹). Thermogravimetric (TGA) curve was carried out on a STA 449 °C Jupiter (NETZSCH) thermogravimetry analyzer from room temperature to 800/1000 °C under air atmosphere with a heating rate of 10 °C min⁻¹. X-ray photoelectron spectroscopy (XPS) characterizations were carried out in an ESCALAB 250 instrument with 150 W Al Kα probe beam.

Electrochemical measurements

The anode electrode slurry for lithium-ion battery was prepared by mixing 70% MoS_2 -N-C powders, 20% carbon black as conductive agent and 10% polyvinylidene fluoride (PVDF) as binder with N-methylpyrrolidone (NMP) dispersion medium, and then coated evenly onto a copper foil (thickness of 10 µm) where the content of active material was around 1 mg cm⁻². A solution of 1 M LiPF₆ dissolved in ethylene carbonate (EC) and dimethyl carbonate (DMC) with a volume ratio of 1:1 was

employed as electrolyte. The coin cells (CR-2025) contained Cellgard 2300 separator and lithium foils asthe counter electrode. The charge-discharge performances were tested galvanostatically in the voltage range of 0.01 to 3.0 V at various current densities using a programmable battery testing system (LAND CT2001A) at 25 °C.



Fig. S1 XRD pattern of 2D Molybdate - dopamine precursor.



Fig. S2 XPS pattern of MoS₂-N-C nanoflake.

The mass content of MoS₂ could be calculated by the equations:

$$m (MoS_2) = m (MoO_3) *M (MoS_2) / M (MoO_3)$$

$$= 49.1\% * 160/144 = 54.56\%$$
(S1)

According to the equations, the mass contents of MoS₂ is 54.56%.

Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %
C1s	284.63	1.71	29389.98	75.84
N1s	397.82	2.99	3181.3	5.08
S2p	931.84	1.47	5082.04	0.98
Mo3d5	231.91	1.22	2846.53	1.11
Ols	532.44	4.6	17421.59	16.99

Table S1- Surface element distribution by XPS

The content of N = (1-54.56%)*(14/(14+12*15))=3.28%

By XPS analyses, the atomic ratio of C and N on the surface of the MoS_2 -N-C is 15:1, presumably, C and N in the whole structure than the same as the 15:1, ignore the influence of oxygen after surface oxidation in the process of test, combined with the result of TG, the content of N in the sample is about 3.28%.



Fig. S3 SEM image of N-C nanoflake.

Sample	Current density (A g ⁻¹)	Maximum stable capacity (mA h g ⁻¹)	Cycle number	Capacity retention (%)	Refer.
ANL MoS2@CNFs	1	802	500	75	Chem. Commun., 2020,56, 141-144
NDG/MoS ₂ /NDG	0.1	600	600	92	Nano Energy. 2017, 41, 154-163
Layered C ₃ N ₄ /NRGO/MoS ₂	0.1	938	100	91	Nano Energy. 2014, 8, 157-164.
MoS ₂ @CMK-3 Nanocomposite	0.25	824	100	73	Nanoscale. 2012, 4, 5868-71
Core-shell MoS ₂	0.1	690	100	94	<i>Small.</i> 2014, 10, 4975-4981.
Quasi-hollow C@MoS ₂	0.1	900	200	91	Journal of Materials Chemistry A. 2016, 4, 10425-10434.
MoS2 Quantum dots-N-C	2 /5 /10	914 /626 /509	500 /600 /1950	80 /75 /51.2	This work

 Table. S2 Summary of electrochemical performances of different MoS₂-based anodes for lithium-ion battery.