

Supporting Information

**FeS Nanosheets Assembled with 1T-MoS₂ Nanoflowers on
Iron Foam for Efficient Overall Water Splitting**

Bo Feng^a, Shuting Jin^b, Jihui Lang^b, Jian Wang^a, Jie Hua^a, Yunfei Sun^a, Wei Zhang^a,
Jin Wang^a, Jian Cao^{*,b}

^aCollege of Information Technology, Jilin Normal University, Siping 136000, PR
China

^bCollege of Physics, Jilin Normal University, Changchun 130103, PR China

Corresponding author E-mail: caojian_928@163.com

1. Experimental

1.1 Materials: All chemicals were used without further purification (analytical grade). Thioacetamide (CH_3CSNH_2) and sodium molybdate dihydrate ($\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$, 99%) were purchased from Shanghai Aladdin Biochemical Technology Co.Ltd (Shanghai, China) and Sinopharm Chemical Reagent Co. Ltd (Shanghai, China).

1.2 Treatment of the Fe foam: A piece of IF (20 mm × 25 mm) was washed with 1 mol/L HCl, acetone, 75% alcohol, and deionized water for several times to clear the surface impurities, and dried at 60 °C for 6 h in vacuum.

1.3 Materials Characterization: X-ray diffraction (XRD) patterns were obtained on a MAC Science MXP-18 X-ray diffractometer utilizing a Cu target radiation source. Transmission electron micrographs (TEM), high-resolution transmission electron micrographs (HRTEM) images were acquired on JEM-2100 electron microscope with the accelerating voltage of 200 kV. The scanning electron microscope (SEM) images, the elemental mappings and energy dispersive X-ray spectroscopy (EDAX) images were obtained on JEOLJ SM-7800F at 10.0 kV. The surface chemistry and the binding energy of different electronic states of the samples were examined by XPS with a Thermo ESCALAB 250Xi.

1.4 Electrochemical Characterization: HER/OER electrochemical performance tests were performed with a CHI 760E electrochemical workstation (Chenhua Corp., Shanghai) in a standard three-electrode system at ambient temperature, of which the graphite rod was used as the counter electrode, the Hg/HgO electrode was worked as the reference electrode and the FMSx sample (cutting into pieces of 0.3×0.3 cm²) was acted as the working electrode. In the two-electrode cell system, the as-prepared FMS_{0.5} was served as cathode and anode respectively for overall water splitting. For comparison, 1T-MoS₂ was dropped on IF for testing, which named as 1T-MoS₂/IF. The electrolyte was 1.0 M KOH (pH = 13.6) for all the electrochemical tests. Before the electrochemical experiments, the electrolyte was previously degassed with N₂ for 30 min. All the potentials were converted to potentials versus the reversible hydrogen electrode (RHE) by using the following equation:

$$E_{RHE} = E_{SCE} + 0.098 + 0.059 \times PH$$

Linear sweep voltammetry (LSV) curves were tested at a scan rate of 5 mV s^{-1} to obtain the polarization curves, which were steady-state after several cycles. All measured polarization curves were iR-corrected. For comparison, commercial Pt/C or RuO_2 were also prepared as working electrodes. In a typical process, 20 mg of the commercial Pt/C (20 wt%) (or RuO_2) powder was dispersed in a mixture of 60 μl of nafion solution (1wt %) and 540 μl of isopropanol solution, which was sonicated for 30 minutes. Then 8 μl of the above solution was dropped on a piece of cleaned IF foam ($0.3 \text{ cm} \times 0.3 \text{ cm}$, catalysts loading $\approx 3 \text{ mg cm}^{-2}$). The cycle durability was measured by the chronoamperometric response. Electrochemical impedance spectroscopy (EIS) measurements were carried out at frequency ranging from 0.1 to 10^4 Hz .

2. Supplementary Results

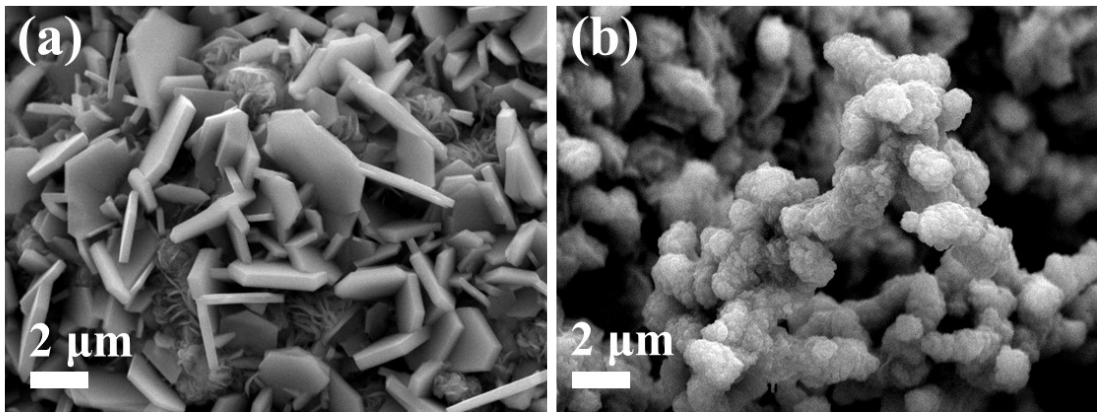


Fig. S1 SEM images of FMS 0.1(a) and FMS 0.9(b)

Table S1. Comparison of HER performance of FMS 0.5 with reported electrocatalysts

Electrolyte	Catalyst	Overpotential (mV)	Current density (mA/cm ²)	Tafel slope (mV/dec ²)	ref
1 M KOH	FeS/Ni ₃ S ₂ @NF	130	10	124	[1]
1 M KOH	CoS ₂ /FeS-MOF@NF-1	137	10	80	[2]
1 M KOH	MoS ₂ @Fe/Ni-MOF ₆₀₀₋₃	140	10	158	[3]
1 M KOH	Ni-1T MoS ₂	199	10	52.7	[4]
1 M KOH	TEA-1T MoS ₂	355	10	70	[5]
1 M KOH	CT _{0.5} -G1	312	10	85	[6]
1 M KOH	1T/2H MoS ₂ (25D) /Ti ₃ C ₂ T _{x-1}	300	10	117.2	[7]
1 M KOH	1T MoS ₂ /GO	209	10	71.7	[8]
1 M KOH	rGO/1T-MoS ₂ /CeO ₂	140	10	43	[9]
1 M KOH	FMS 0.5	245	100	80.6	This work

Table S2. Comparison of OER performance of FMS 0.5 with reported electrocatalysts

Electrolyte	Catalyst	Overpotential (mV)	Current density (mA/cm ²)	Tafel slope (mV/dec ²)	ref
1 M KOH	FeS/Ni ₃ S ₂ @NF	192	10	70	[1]
1 M KOH	CoS ₂ /FeS-MOF@NF- 1	244	50	27	[2]
1 M KOH	MoS ₂ @Fe/Ni-MOF ₆₀₀₋₃	340	10	158	[3]
1 M KOH	Ni-1T MoS ₂	310	10	103.2	[4]
1 M KOH	FeS/Fe ₃ C@N-S-C-800	570	10	81	[10]
1 M KOH	1T-Ni _{0.2} Mo _{0.8} S _{1.8} P _{0.2} NS/CC	305	40	76.5	[11]
1 M KOH	0.2-A@NF	190	10	166	[12]
1 M KOH	NiFe LDH/MoS ₂	190	10	31	[13]
1 M KOH	NiFe ₂ O ₄ /MoS ₂	280	10	48.7	[14]
1 M KOH	MoS ₂ /NiS ₂ /CC-2	384	100	58	[15]
1 M KOH	FMS 0.5	316	100	88.3	This work

Table S3. The charge transfer resistance of IF, FeS, 1T-MoS₂/IF and FMSx

Samples	IF	FeS	1T MoS₂/IF	FMS0.1	FMS0.5	FMS0.9
R _{ct} (Ω) HER	1.92	1.1	1.43	0.9	0.72	0.93
R _{ct} (Ω) OER	1.15	1	0.98	0.7	0.65	0.71

References

- [1] H. Li, S. Yang, W. Wei, M. Zhang, Z. Jiang, Z. Yan, J. Xie, Chrysanthemum-like FeS/Ni₃S₂ heterostructure nanoarray as a robust bifunctional electrocatalyst for overall water splitting, *Journal of Colloid and Interface Science*, 2022, 608, 536-548.
- [2] Y. Yang, Q. Zhou, J. Yang, D. Qian, Y. Xiong, Z. Li, Z. Hu, Metal-organic framework derived CoS₂/FeS-MOF with abundant heterogeneous interface as bifunctional electrocatalyst for electrolysis of water, *International Journal of Hydrogen Energy*, 2022, 47, 33728-33740.
- [3] Z. Lin, T. Feng, X. Ma, G. Liu, Fe/Ni bi-metallic organic framework supported 1T/2H MoS₂ heterostructures as efficient bifunctional electrocatalysts for hydrogen and oxygen evolution, *Fuel*, 2023, 339, 127395.
- [4] G. Wang, G. Zhang, X. Ke, X. Chen, X. Chen, Y. Wang, G. Huang, J. Dong, S. Chu, M. Sui, Direct synthesis of stable 1T-MoS₂ doped with Ni single atoms for water splitting in alkaline media, *Small*, 2022, 18, 2107238.
- [5] A. S. Goloveshkin, N. D. Lenenko, M. I. Buzin, V. I. Zaikovskii, A. V. Naumkin, A. S. Golub, Organic interlayers boost the activity of MoS₂ toward hydrogen evolution by maintaining high 1T/2H phase ratio, *International Journal of Hydrogen Energy*, 2023, 48, 10555-10565.
- [6] Y. Zhao, X. Zhang, T. Wang, T. Song, P. Yang, Fabrication of rGO/CdS@2H, 1T, amorphous MoS₂ heterostructure for enhanced photocatalytic and electrocatalytic activity, *International Journal of Hydrogen Energy*, 2020, 45, 21409-21421.
- [7] J. Y. Loh, F. M. Yap, W. J. Ong, 2D/2D heterojunction interface: Engineering of 1T/2H MoS₂ coupled with Ti₃C₂T_x heterostructured electrocatalysts for pH-universal hydrogen evolution, *Journal of Materials Science & Technology*, 2024, 179, 86-97.
- [8] Y. Lv, H. Pan, J. Lin, Z. Chen, Y. Li, H. Li, M. Shi, R. Yin, S. Zhu, One-pot hydrothermal approach towards 2D/2D heterostructure based on 1T MoS₂ chemically bonding with GO for extremely high electrocatalytic performance, *Chemical Engineering Journal*, 2022, 428, 132072.
- [9] K. Nie, X. Qu, D. Gao, B. Li, Y. Yuan, Q. Liu, X. Li, S. Chong, Z. Liu, Engineering phase stability of semimetallic MoS₂ monolayers for sustainable

electrocatalytic hydrogen production, *ACS Applied Materials & Interfaces*, 2022, 14, 19847-19856.

[10] F. Kong, X. Fan, A. Kong, Z. Zhou, X. Zhang, Y. Shan, Covalent phenanthroline framework derived FeS@Fe₃C composite nanoparticles embedding in N-S-Codoped carbons as highly efficient trifunctional electrocatalysts, *Advanced Functional Materials*, 2018, 28, 1803973.

[11] U. N. Pan, T. I. Singh, D. R. Paudel, C. C. Gudal, N. H. Kim, J. H. Lee, Covalent doping of Ni and P on 1T-enriched MoS₂ bifunctional 2D-nanostructures with active basal planes and expanded interlayers boosts electrocatalytic water splitting, *Journal of Materials Chemistry A*, 2020, 8, 19654-19664.

[12] Y. Zhao, S. Wei, F. Wang, L. Xu, Y. Liu, J. Lin, K. Pan, H. Pang, Hatted 1T/2H-phase MoS₂ on Ni₃S₂ nanorods for efficient overall water splitting in alkaline media, *Chemistry—A European Journal*, 2020, 26, 2034-2040.

[13] S. Chakraborty, S. Marappa, S. Agarwal, D. Bagchi, A. Rao, C.P. Vinod, S.C. Peter, A. Singh, M. Eswaramoorthy, Improvement in oxygen evolution performance of NiFe layered double hydroxide grown in the presence of 1T-rich MoS₂, *ACS Applied Materials & Interfaces*, 2022, 14, 31951-31961.

[14] M. M. Sebastian, P. Velayudham, A. Schechter, N. Kalarikkal, Spinel nickel ferrite nanoparticles supported on a 1T/2H mixed-phase MoS₂ heterostructured composite as a bifunctional electrocatalyst for oxygen evolution and oxygen reduction reactions, *Energy & Fuels*, 2022, 36, 7782-7794.

[15] J. Xu, J. Rong, Y. Zheng, Y. Zhu, K. Mao, Z. Jing, T. Zhang, D. Yang, F. Qiu, Construction of sheet-on-sheet hierarchical MoS₂/NiS₂ heterostructures as efficient bifunctional electrocatalysts for overall water splitting, *Electrochimica Acta*, 2021, 385, 138438.