Supplementary Materials

N, P co-doping triggered phase transition of MoS_2 with enlarged interlayer spacing for efficient hydrogen evolution

Ailing Feng[a] ,Shijiu Ding[a], Peitao Liu*[,a], Yanqing Zu[a], Fengbo Han[a], Xiaodong Li[a], Liang Liu[a] and Yanan Chen[a]

[a] Institute of Physics & Optoelectronics Technology, Baoji University of Arts and Sciences, Baoji, 721016, China

Corresponding author: Tel: 0917-3627689; E-mail: liupt@bjwlxy.edu.cn

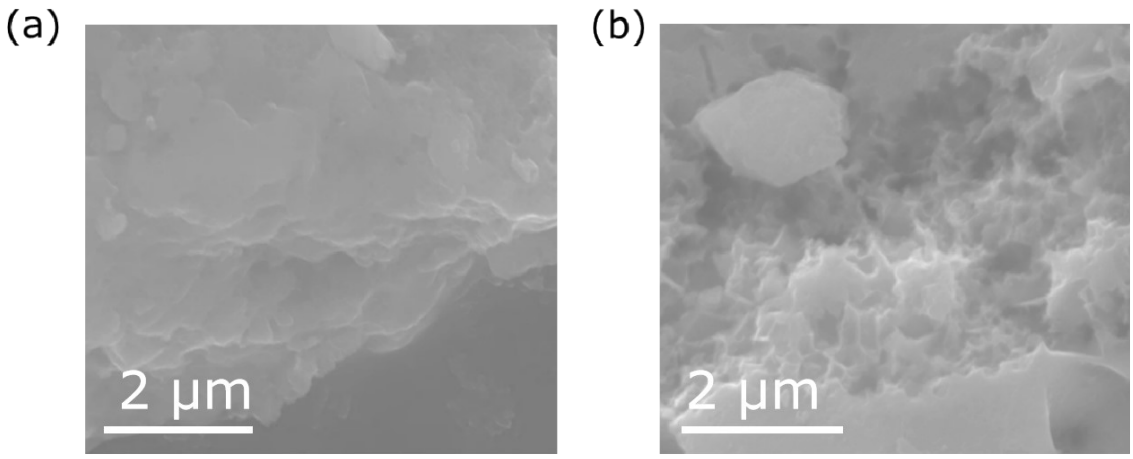

Figure S1. (a) SEM results of N-MoS_2 and (b) N, P co-doped MoS_2 nanosheet.

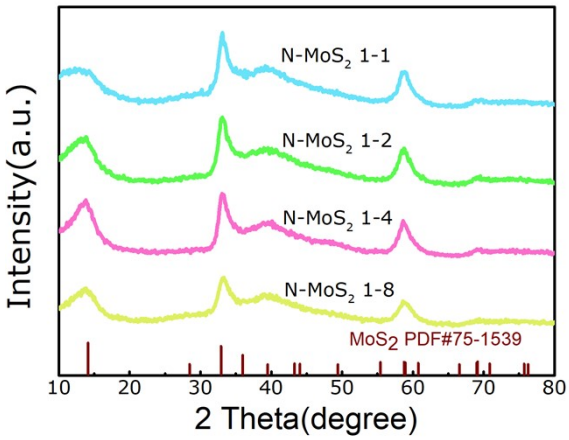

Figure S2. XRD results of N-MoS_2 1-1, N-MoS_2 1-2, N-MoS_2 1-4 and N-MoS_2 1-8.

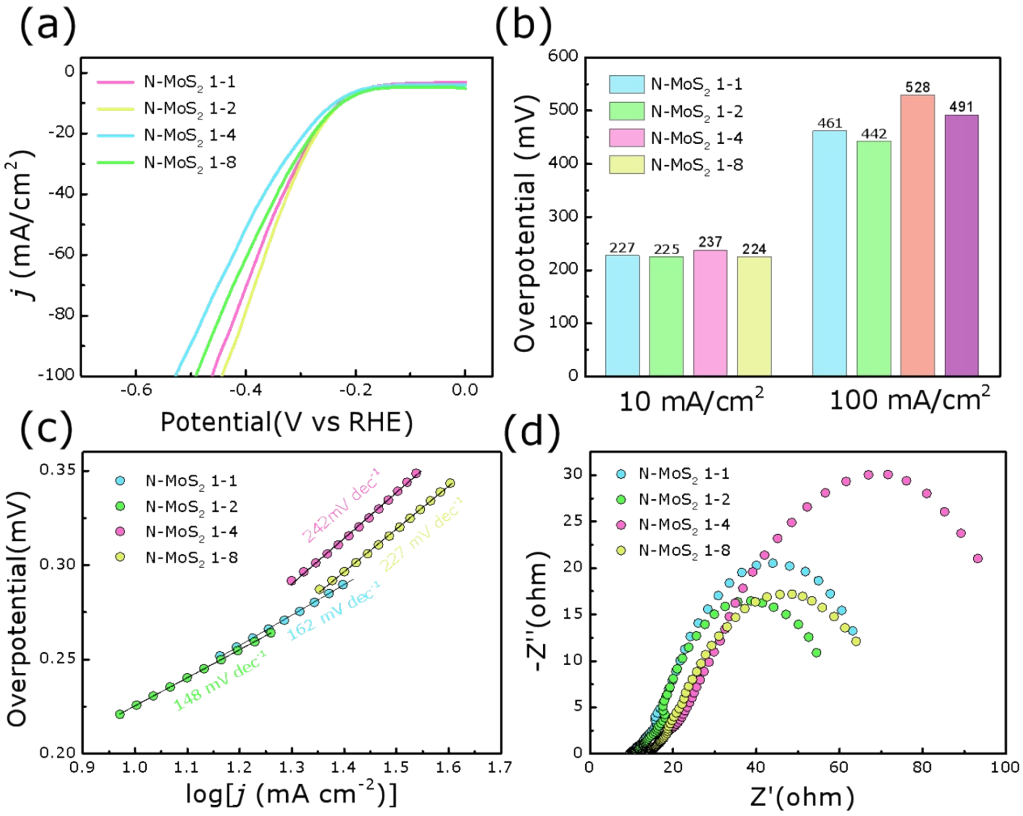

Figure S3. Electrochemical Test Diagram of N-MoS_2. (a) The LSV curves, (b) the overpotential, (c) the corresponding Tafel slope, and (d) the electrochemical impedance of N-MoS_2 1-1, N-MoS_2 1-2, N-MoS_2 1-4 and N-MoS_2 1-8.

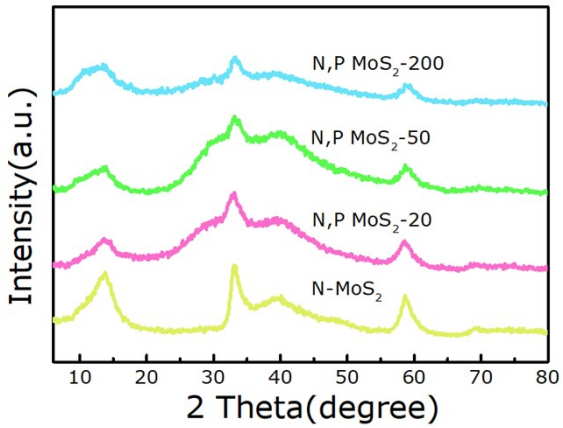

Figure S4. XRD results of N-MoS_2, N, P-MoS_2-20, N, P-MoS_2-50 and N, P-MoS_2-200.

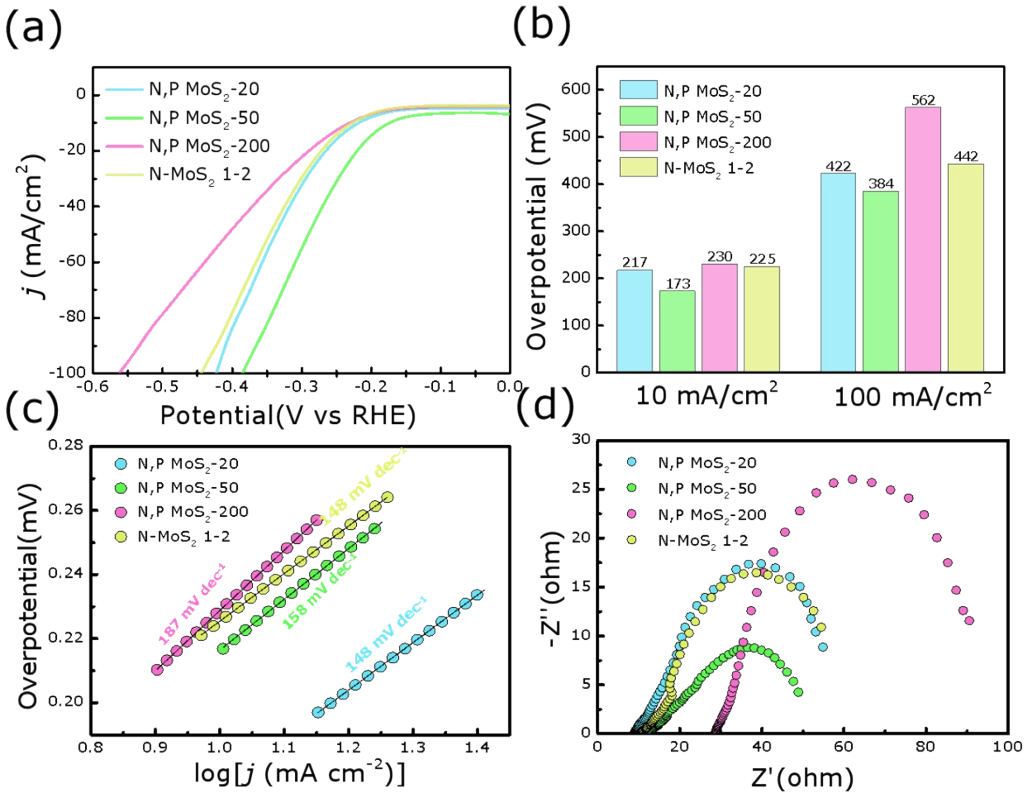

Figure S5. Electrochemical Test Diagram of N, P-MoS_2. (a) The LSV curves, (b) the overpotential, (c) the corresponding Tafel slope, and (d) the electrochemical impedance of N-MoS_2 1-2, N, P-MoS_2-20, N, P-MoS_2-50, N, P-MoS_2-200.

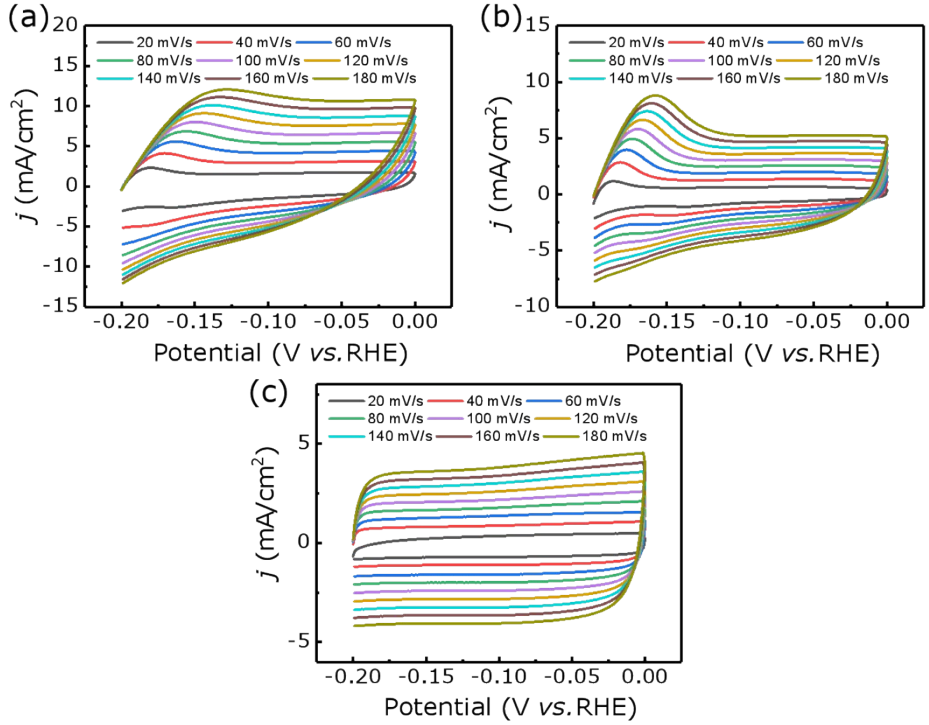

Figure S6. Electrochemical capacitance measurements were performed to determine the ECSA of (a) Pt/C, (b) N, P-MoS_2 and (c) N-MoS_2.

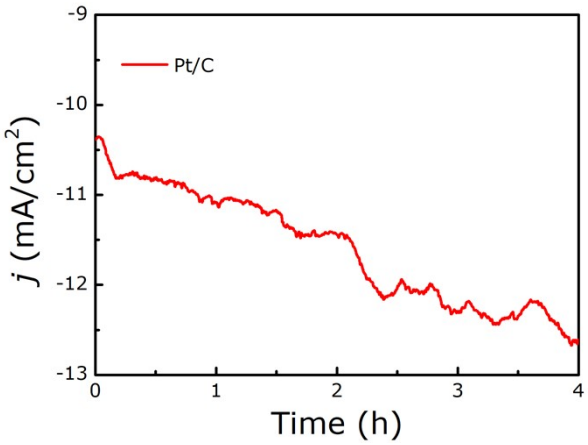

Figure S7.*i-t* curves of commercial Pt/C.

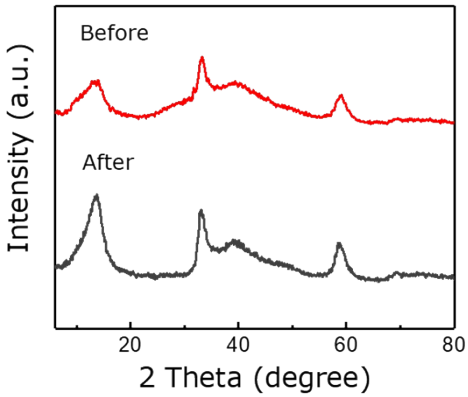

Figure S8. The XRD results for the N, P-MoS_2 before and after HER activity.

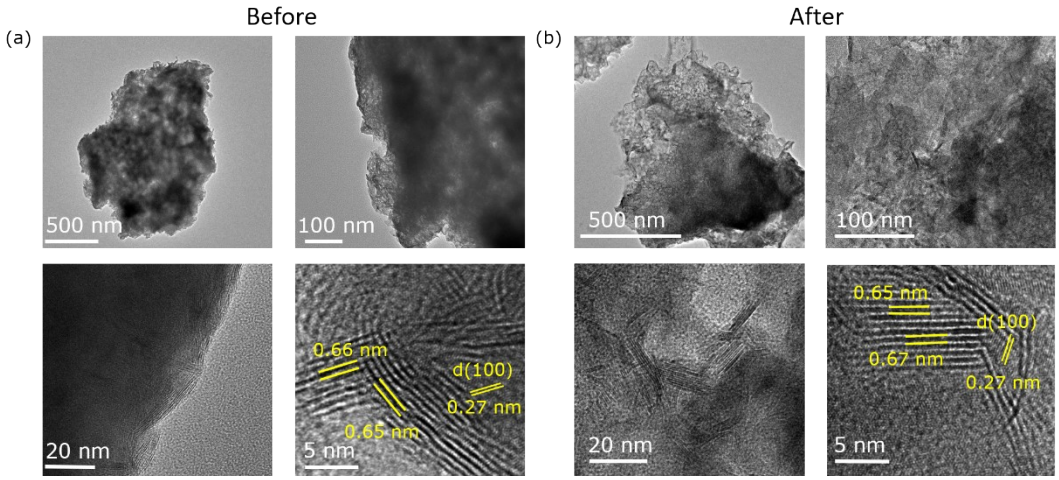

Figure s9. (a)-(b) The TEM and HRTEM results for the N, P-MoS_2 before and after HER activity.

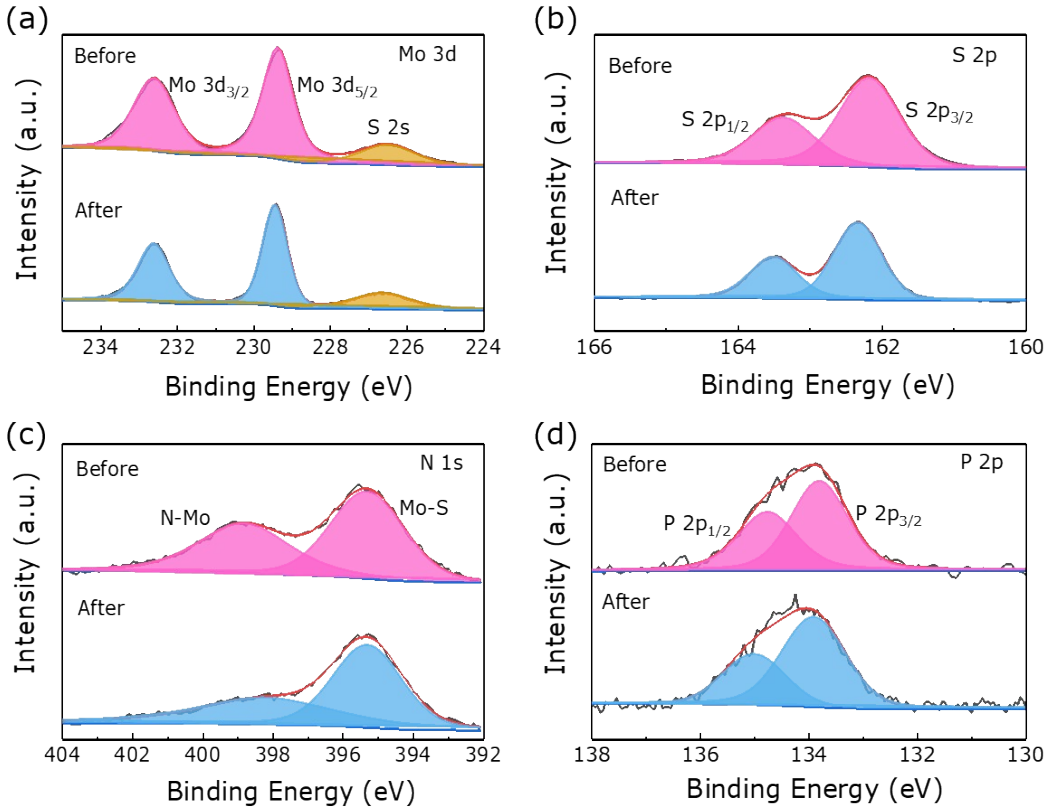

Figure S10. (a) The Mo 3d XPS spectrum, (b) S 2p XPS spectrum, (c) N 1s XPS, and (f) P 2p XPS spectrum of the N, P-MoS_2 before and after HER activity.

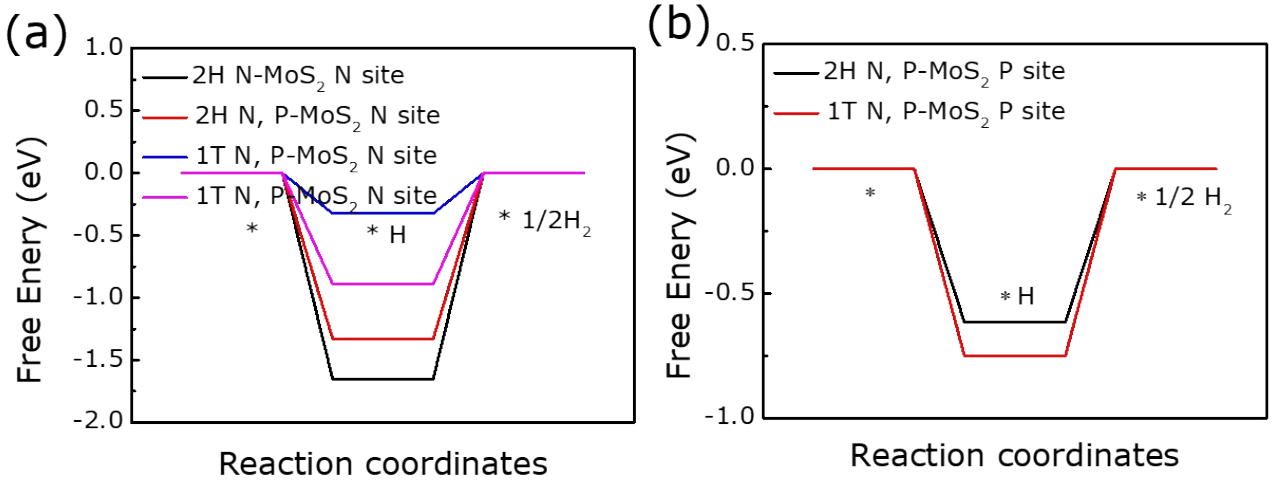

Figure S11. (a) The free energy diagram for HER on 2H N-MoS_2, 2H N, P-MoS_2, IT N-MoS_2, and 1T N, P-MoS_2 N sites, respectively. (b) The free energy diagram for HER on 2H N, P-MoS_2 and 1T N, P-MoS_2 P sites, respectively.

Table S1. Comparison of the HER performances of N, P-MoS_2 with some of the previously reported MoS_2-based catalysts.

Catalyst	Electrolytes	Potential	η	Reference
N, P-MoS_2	0.5 M H_2SO_4	179 mV	10 mA/cm^2	This work
MoS_2/graphite	0.5 M H_2SO_4	183 mV	10 mA/cm^2	[1]
Zn@MoS_2	0.5 M H_2SO_4	194 mV	10 mA/cm^2	[2]
1T/2H-MoS_2 nanosheets	0.5 M H_2SO_4	220 mV	10 mA/cm^2	[3]
Monolayer MoS_2	0.5 M H_2SO_4	160 mV	10 mA/cm^2	[4]
1T-MoS_2 ultra-thin flakes	0.5 M H_2SO_4	254 mV	10 mA/cm^2	[5]
EA-2H/1T/RGO	0.5 M H_2SO_4	186 mV	10 mA/cm^2	[6]
O-MoS_2/G	0.5 M H_2SO_4	200 mV	20 mA/cm^2	[7]
O, P-MoS_2	0.5 M H_2SO_4	277 mV	50 mA/cm^2	[8]
Co_9S_8/NC@MoS_2	1 M PBS	261 mV	10 mA/cm^2	[9]
MoP	1 M PBS	187 mV	10 mA/cm^2	[10]
Co_9S_8@MoS_2/CNFs	0.5 M H_2SO_4	190 mV	10 mA/cm^2	[11]

Notes and references

1. C. C. Cheng, A. Y. Lu, C. C. Tseng, X. Yang, M. N. Hedhili, M. C. Chen, L. J. Li, *Nano Energy*, 2016, **30**, 846-852.
2. W. Wu, C. Niu, C. Wei, Y. Jia, C. Li, Q. Xu, *Angew. Chem. Int. Edit.*, 2019, **58**, 2029-2033.
3. Z. Liu, Z. Gao, Y. Liu, M. Xia, R. Wang, N. Li, *ACS Appl. Mater. Inter.*, 2017, **9**, 25291-25297.
4. Y. Xu, L. Wang, X. Liu, S. Zhang, C. Liu, D. Yan, S. Luo, *J. Mater. Chem. A* , 2016, **4**, 16524-16530.

5. F. Yang, Z. F. Cao, J. Wang, S. Wang, H. Zhong, *Int. J. Hydrogen. Energ.*, 2019, **44**, 21229-21237.

6. K. Zhang, B. Jin, Y. Gao, S. Zhang, H. Shin, H. Zeng, J. H. Park, *Small*, 2019, **15**, 1804903.

7. J. Guo, F. Li, Y. Sun, X. Zhang, L. Tang, *J. Power Sources*, 2015, **291**, 195-200.

8. J. Liu, Z. Wang, J. Li, L. Cao, Z. Lu, D. Zhu, *Small*, 2020, **16**, 1905738.

9. H. Li, X. Qian, C. Xu, S. Huang, C. Zhu, X. Jiang, L. Hou, *ACS Appl. Mater. Inter.* , 2017, **9**, 28394-28405.

10. B. Kim, T. Kim, K. Lee, J. Li, *ChemElectroChem*, 2020, **7**, 3578-3589.

11. H. Zhu, J. Zhang, R. Y. zhang, M. Du, Q. Wang, G. Gao, X. Zhang, Adv. Mater., 2015, **27**, 4752-4759.