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Single-Crystal Nitrogen-Rich 2D Mo<sub>5</sub>N<sub>6</sub> Nanosheets for **Efficient and Stable Seawater Splitting** 

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## Abstract

- Seawater is the most abundant water source and electrolyte for low-cost hydrogen production.<sup>1, 2</sup>
- > However, the stability of most electrocatalysts for hydrogen evolution reaction (HER) in seawater is poor due to the highly corrosive environment.<sup>3, 4</sup>

# **HER Performance and Activity Origin**

- > Excellent HER activity and stability in seawater.
- $\succ$  The *d* band center position of Mo<sub>5</sub>N<sub>6</sub> is close to Pt.



> Nitrogen—rich metal nitrides (N/metal > 1) such as  $Mo_5N_6$  are preferable for seawater splitting because of their good corrosion resistance and high activity.<sup>4</sup>



Figure 1. Schematic of the synthesis of Mo<sub>5</sub>N<sub>6</sub> nanosheets.

#### Highlights

- $\blacktriangleright$  Nitrogen-rich 2D Mo<sub>5</sub>N<sub>6</sub> single-crystal nanosheets are synthesized for the first time.<sup>5</sup>
- Excellent HER performance in pH universal electrolytes including natural seawater.
- $\succ$  The performance of 2D Mo<sub>5</sub>N<sub>6</sub> for seawater splitting is better than the commercial Pt/C benchmark.

## **Materials Characterization**

- $\succ$  Morphology of 2D Mo<sub>5</sub>N<sub>6</sub>.
- $\geq$  Electronic structure of 2D Mo<sub>5</sub>N<sub>6</sub>.





225

- -10 Pt  $Mo_5N_6$ MoN Energy (eV) Figure 3. (a-d) Comparison of HER performance in seawater with
- other TMNs and Pt/C in seawater conditions. (e) DOS of  $Mo_5N_6$ . (f) d band centre position of Pt (111),  $Mo_5N_6$  and MoN.

## Conclusion

- $\succ$  The HER performance of 2D Mo<sub>5</sub>N<sub>6</sub> in natural seawater is better than Pt/C benchmark.
- > Excellent stability in seawater splitting with over 80% of its initial current retention for 100 h test.
- $\succ$  The high Mo valence state in Mo<sub>5</sub>N<sub>6</sub> enhanced its corrosive-resistance.

#### References

1. W. Tong, et al., *Nat. Mater.*, **5**, 367 (2020). 2. X. Lu, et al., Energy Environ. Sci., 11, 1898 (2018).

Figure 2. (a-c) Transmission electron microscopy analysis of  $Mo_5N_6$ . (c) Mo 3d XPS spectra of MoN and  $Mo_5N_6$ .

3. H. Jin, et al., *Chem. Rev.*, **118**, 6337 (2018). 4. L. Yu, et al., *Nat. Commun.*, **10**, 5106 (2019). 5. H. Jin, et al., ACS Nano, 12, 12761 (2018).

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