Development of Nitride MXene-Based Nanocomposites as Next-Generation Oxygen Evolution Electrocatalysts for Water Splitting

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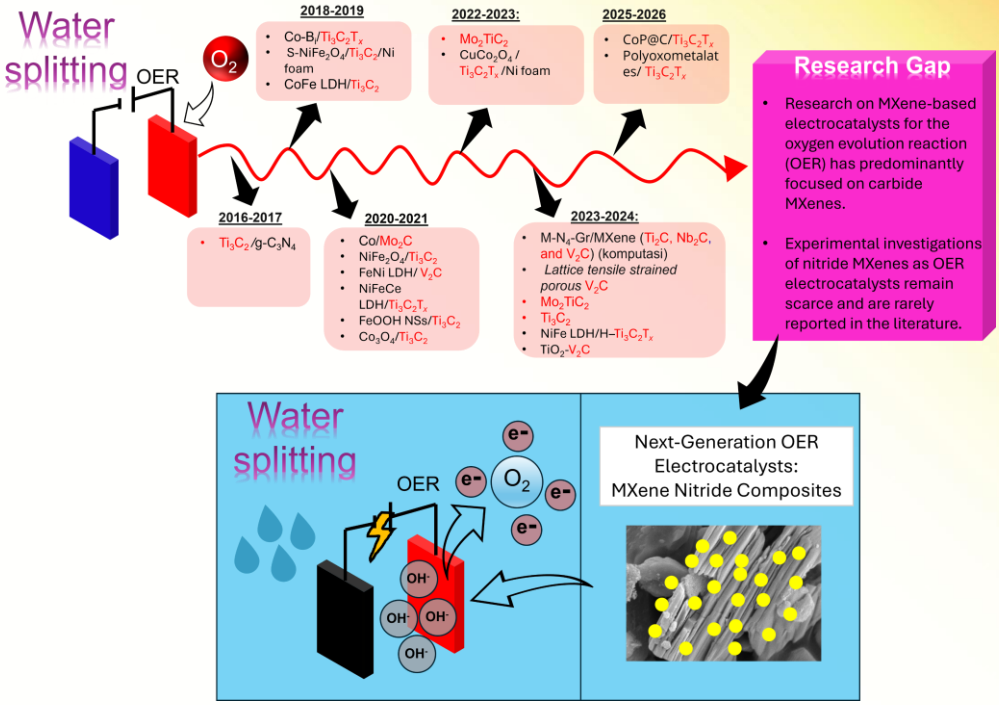
Abstract

Water splitting via electrolysis offers a sustainable route to hydrogen production. However, its efficiency is limited by the oxygen evolution reaction (OER). This reaction is kinetically sluggish, requires a high overpotential, and demands catalysts that remain stable under oxidative conditions. While precious metals still dominate OER electrocatalysis, their cost and scarcity have shifted attention toward non-precious transition-metal alternatives. These materials, however, suffer from low electrical conductivity. Hybridizing them with MXene, a two-dimensional (2D) transition metal carbide/nitride known for its excellent conductivity and charge transfer, offers a way to overcome this limitation.

Herein, we developed a composite of Ti_2N MXene and nanoporous NiO, deposited on a glassy carbon electrode (GCE) and evaluated for the OER and the hydrogen evolution reaction (HER). The composite exhibited a lower overpotential than either component, and Density Functional Theory (DFT) calculations revealed more favorable adsorption energies, confirming the benefit of combining the two materials.

Keyword: Clean energy, Electrocatalysis, Ti_2N, Nanoporous NiO

Introduction



Method

❑ Synthesis of Ti_2N MXene

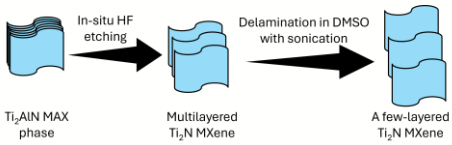


Figure 1. Illustration of the MXene synthesis procedure

❑ Synthesis of Nanoporous n-NiO

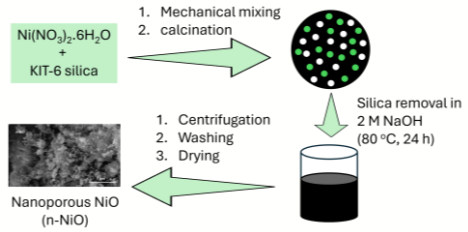


Figure 2. Illustration of the n-NiO synthesis procedure

❑ Preparation of GCE/Ti_2N MXene/n-NiO electrode

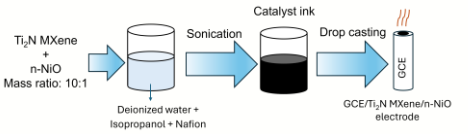
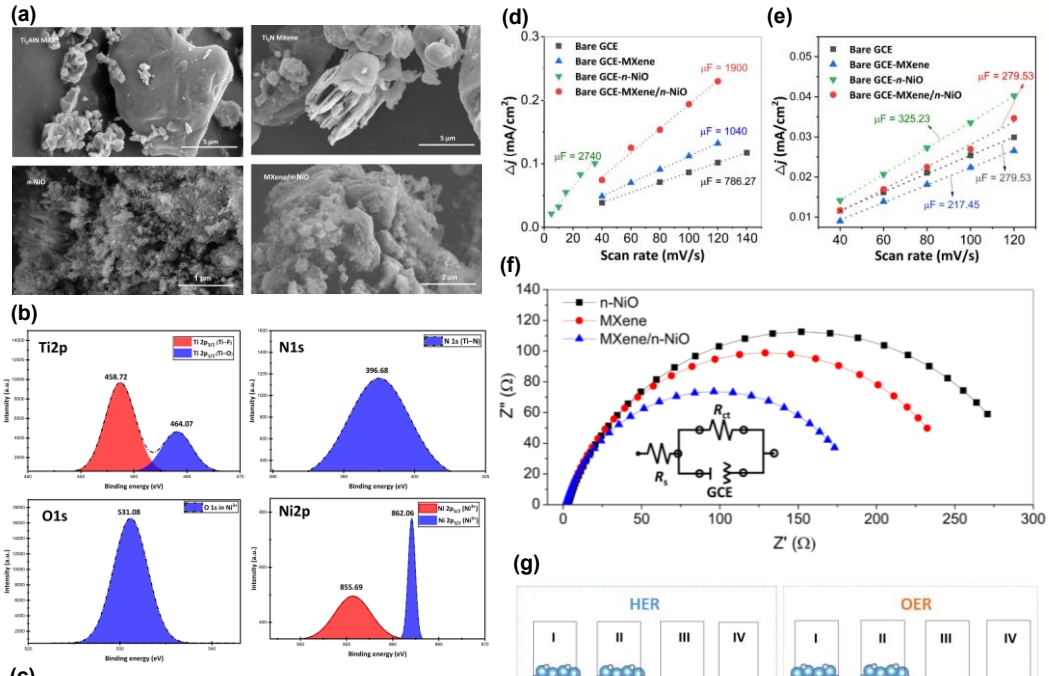


Figure 3. Illustration of the GCE/Ti_2N MXene/n-NiO electrode preparation procedure

❑ Characterization

Structural characterization was performed using XRD, SEM, TEM, and XPS, while textural properties were analyzed by N_2 adsorption-desorption. Electrocatalytic performance toward HER and OER was evaluated using LSV, CV, and EIS

Results and Discussions



(c)

	Ti_2N	n-NiO	Ti_2N/n-NiO
S_{BET} (m^2/g)	40	129	55
S_{EXT} (m^2/g)	37.2	113.6	55.4
V_{total} (cm^3/g)	0.855	0.749	0.424
V_{mikro} (cm^3/g)	0.085	0.733	0.401

Figure 4. (a) SEM images of MAX, MXene, n-NiO, and MXene/n-NiO; (b) XPS spectra of MXene/n-NiO; (c) pore characteristics; double-layer capacitance for (d) HER in 0.5 M H_2SO_4 and (e) OER in 1.0 M KOH; (f) Nyquist plots; (g) Gibbs free energies of H* and O* adsorption (ΔG_{H^*}, ΔG_{O^*}) with schematic adsorption configurations.

Conclusion

Novel Ti_2N MXene/n-NiO nanocomposites have been successfully synthesized with improved electrochemical behavior compared to their components. This study offers a promising strategy for developing an enhanced electrocatalyst for sustainable hydrogen production.