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INVESTIGATING MXENE MATERIAL FOR EVOLUTION REACTION IN WATER SPLITTING

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Abstract: We report a MXene-based hierarchical electrode architecture specifically engineered to address these challenges for alkaline OER. A $\text{Ti}_3\text{C}_2\text{T}_x$ MXene/Nickel Foam (MXene/NF) electrode is fabricated via a simple immersion strategy, enabling intimate interfacial coupling between highly conductive MXene nanosheets and a three-dimensional porous nickel scaffold. This architecture achieves an OER overpotential of 360 mV at 10 mA cm^{-2} and exhibits stable operation at 100 mA cm^{-2} , indicating efficient charge-transfer kinetics and mechanical robustness. To further mitigate MXene restacking and enhance mass transport, graphene oxide (GO) is incorporated as structural spacers and conductive bridges, yielding a MXene@GO composite with a reduced OER overpotential of 290 mV and improved thermodynamic efficiency. Electrochemical analyses reveal a significantly increased electrochemically active surface area and sustained catalytic performance during prolonged operation. This work demonstrates that hierarchical engineering of MXene-based composites provides an effective and scalable strategy for high-performance OER electrocatalysis in alkaline water-splitting systems.

Keywords: Catalyst, MXene, Water splitting, Electrochemistry.

Introduction. Sustainable energy system has intensified interest in green hydrogen as a clean and versatile energy carrier capable of supporting decarbonization across industrial, transportation, and power-generation sectors [1-3]. Among available hydrogen production routes, alkaline water electrolysis remains one of the most mature and scalable technologies due to its operational safety, long-term stability, and compatibility with non-precious metal catalysts [4-5]. However, the overall efficiency of alkaline electrolyzers is fundamentally limited by the sluggish kinetics [6] of the oxygen evolution reaction (OER), which requires a complex four-electron transfer process and accounts for the majority of the energy losses in water splitting.

Nickel-based materials are regarded as benchmark OER catalysts in alkaline media owing to their favorable adsorption energetics for oxygen intermediates, good electrical conductivity, and economic viability [7-10]. In particular, nickel foam (NF) has attracted considerable attention as a three-dimensional conductive scaffold because of its high porosity, interconnected architecture, and mechanical robustness, which facilitate electrolyte penetration and gas release. Nevertheless, bare nickel-based electrodes often suffer from limited active-site density and suboptimal charge-transfer kinetics, motivating the integration of advanced functional materials to enhance their catalytic performance [11,12]. Two-dimensional (2D) materials have emerged as promising candidates for electrocatalysis due to their high surface-to-volume ratio and tunable electronic structures. Among them, MXenes—a family of transition metal carbides and nitrides derived from MAX phases—have attracted increasing interest in electrochemical

applications. $\text{Ti}_3\text{C}_2\text{T}_x$ MXene, in particular, exhibits metallic conductivity, hydrophilic surfaces, and abundant surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$), which can modulate adsorption energies of reaction intermediates and facilitate electron transfer. These properties make MXenes attractive platforms for OER catalysis, especially when integrated with conductive substrates [13-15].

Despite these advantages, practical application of MXene-based OER electrodes remains constrained by several intrinsic challenges, including nanosheet restacking, limited mass transport, and structural instability under prolonged oxidative potentials. Restacking of MXene layers reduces electrochemically active surface area, while insufficient ion diffusion pathways hinder reaction kinetics at high current densities. Therefore, rational architectural engineering is essential to fully exploit the catalytic potential of MXenes in alkaline OER systems [16,17].

Herein, we report a hierarchical MXene-based electrode system specifically designed to enhance OER performance in alkaline water electrolysis. A $\text{Ti}_3\text{C}_2\text{T}_x$ MXene/Nickel Foam (MXene/NF) electrode is fabricated via a simple immersion method, ensuring intimate interfacial contact between MXene nanosheets and the porous nickel scaffold. Furthermore, a MXene@GO composite electrode is developed to suppress MXene restacking and optimize charge and mass transport. The electrochemical performance, kinetics, active surface area, and long-term stability of these electrodes are systematically evaluated, demonstrating the effectiveness of hierarchical MXene composite engineering as a scalable strategy for high-performance OER electrocatalysis.

Results and discussion. Figure 1 presents a comprehensive electrochemical analysis of MXene/NF and MXene-GO- CB/NF electrodes for water splitting. Figure 1(a) shows the chronoamperometric stability test of MXene/NF electrode at 100 mA/cm^2 , where the stable potential over 14 hours indicates robust structural integrity and excellent long-term durability, essential for practical electrolyzer applications. The polarization curve in Figure 1(b) demonstrates the oxygen evolution reaction (OER) performance of MXene/NF, revealing an overpotential of 360 mV, while MXene@GO shows 290 mV which suggests efficient oxygen evolution facilitated by its high electrical conductivity and surface-active sites. The polarization curve shows an OER onset potential around 1.5 V vs. RHE with a gradual increase in current density beyond this point, indicating active oxygen evolution. For Tafel slope calculation from the linear sweep voltammetry (LSV) data, the overpotential (η) was obtained by subtracting the reaction's thermodynamic potential from each applied potential, with current density (j) values extracted from the LSV. The Tafel slope, which offers insight into the reaction mechanism, was determined by plotting overpotential against the logarithm of current density following the equation:

$$\eta = b \log j + a$$

where b is the Tafel slope, typically expressed in mV/dec. Higher Tafel slope values often indicate a one-electron transfer rate-limiting step, while lower values suggest faster kinetics or differing rate determining steps.

Figures 1c illustrate the Tafel slopes, where MXene/NF shows values of 180 mV/dec for OER, indicating effective charge transfer and reaction kinetics. However, the Tafel slopes for MXene@GO are higher (382 mV/dec for OER), indicating slower charge transfer process. The observations can be attributed to electron density distribution and interfacial interactions, where MXene's metallic conductivity ensures rapid charge mobility, while GO and CB enhance the exposure of active sites. MXene's surface functional groups (-OH, -F, -O) contribute to its catalytic behavior, influencing intermediate adsorption and reaction pathways. The presence of GO and CB in MXene@GO enhances the catalytic activity by increasing active surface area and promoting mass transport, making it a favorable electrode for reducing overpotential, while MXene/NF excels in rapid charge transfer and kinetic efficiency.

The thermodynamic efficiency, considering $FE=1$, of the process was calculated and found to be 82% under standard conditions for MXene/NF electrode and 88% for MXene-GO-CB/NF electrode, indicating the ratio of useful energy output relative to the total energy input. This efficiency value reflects how effectively the system converts the supplied energy into the desired chemical or electrical output under these controlled conditions. Achieving high thermodynamic efficiency is crucial as it directly impacts the system's overall energy economy and sustainability.

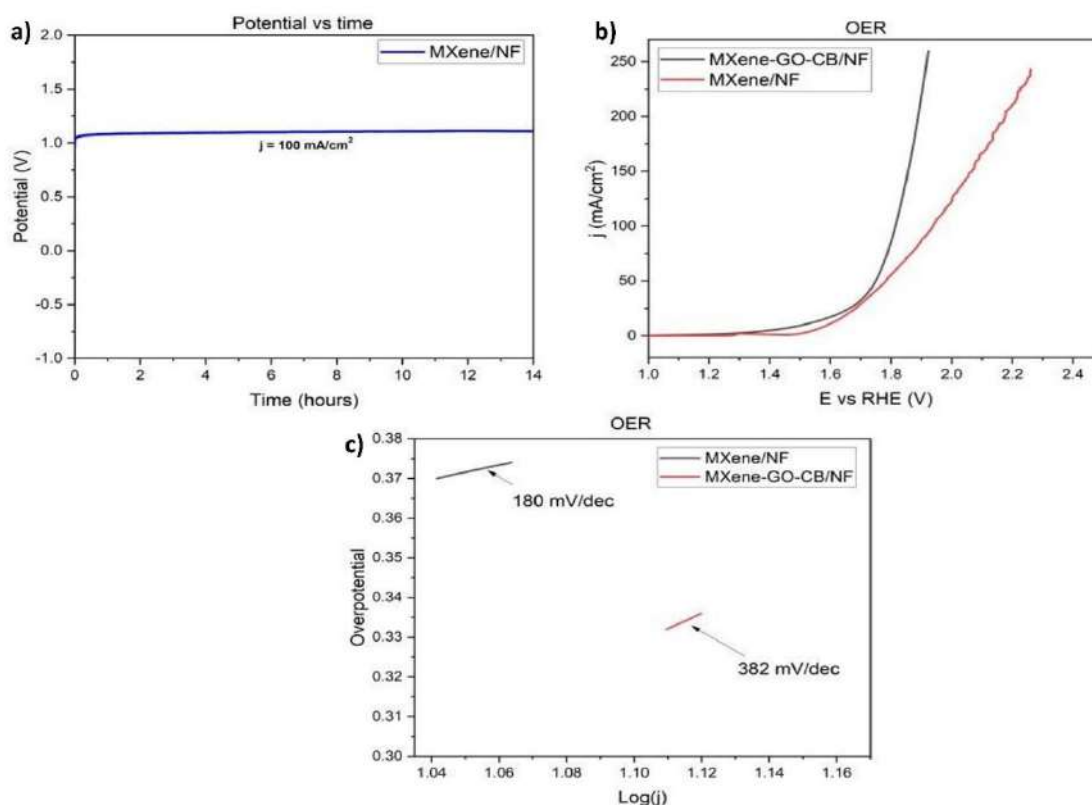


Fig. 1. Electrochemical performance of MXene-based electrodes for the OER and HER. (a) Chronopotentiometry test at 100 mA/cm^2 , showing the potential stability over time. (b) Linear sweep voltammetry (LSV) curves comparing MXene/NF and MXene@GO electrodes. (d) Tafel plots

The Electrochemically Active Surface Area (ECSA) is a fundamental parameter in electrocatalysis that represents the portion of an electrode's surface that actively participates in electrochemical reactions. Unlike the geometrical surface area, which only accounts for the physical dimensions of the electrode, the ECSA reflects the real number of exposed catalytic sites available for charge transfer. A higher ECSA generally translates to improved electrocatalytic efficiency, as it increases the number of available reaction sites for key processes such as the OER and the HER.

The double-layer capacitance, C_{dl} , is a parameter that represents the capacitance of the electrical double layer formed at the interface between the electrode surface and the electrolyte solution. When a potential is applied to the electrode, ions from the electrolyte are attracted to the surface, creating a double layer of charges with a capacitance that depends on the surface area of the electrode.

To determine the electrochemical surface area (ECSA), the double-layer capacitance (C_{dl}) is initially derived from cyclic voltammetry (CV) measurements in the non-faradaic region. This is achieved by plotting the average current density against the scan rate, where the resulting slope corresponds to the C_{dl} value. Figure 2a presents cyclic voltammetry (CV) curves for the MXene/Nickel Foam (NF) electrode recorded at various scan rates (1, 2, 3, 4, and 5 mV/s). These curves illustrate the capacitive behavior of the electrode in the non-faradaic region, confirming the formation of an electrochemical double layer. The gradual increase in current density with increasing scan rate indicates enhanced charge storage capabilities and surface area exposure. To estimate C_{dl} , the linear fitting of $\Delta j/2$ versus scan rate is plotted in Figure 2b, revealing a capacitance value of 202 mF/cm² for OER. This relatively high C_{dl} suggests that the MXene/NF composite offers a large active surface area, which can facilitate charge accumulation and improve reaction kinetics during water oxidation.

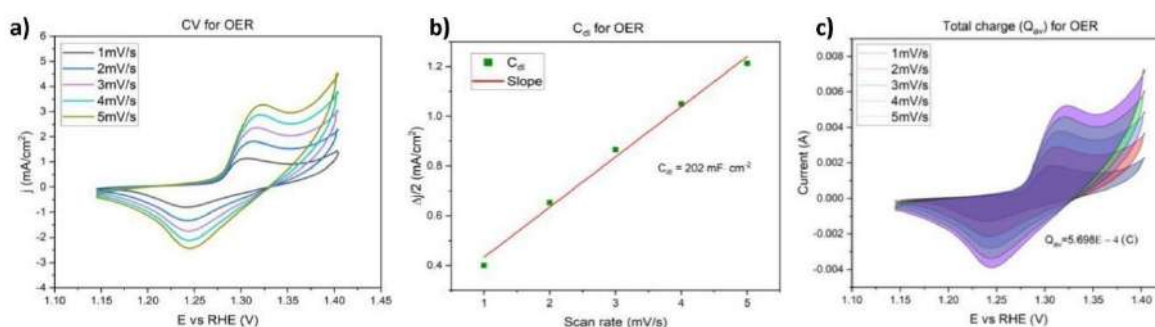


Fig. 2. Electrochemical characterization of the MXene/Nickel Foam (NF) electrode for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). (a) Cyclic voltammetry (CV) curves for OER at different scan rates (1–5 mV/s), used to estimate the electrochemical double-layer capacitance (C_{dl}). (b) Linear fitting of $\Delta j/2$ vs. scan rate for OER. (c) Total charge (Q_{av}) extracted from CV curves for OER

A consistent and reliable C_s value is essential. The specific capacitance, C_s , represents the intrinsic capacitance per unit area of a material in a given electrolyte, and

it can vary based on the electrode material and electrolyte conditions. To determine C_s , cyclic voltammetry (CV) plots of current versus potential were analyzed at different scan rates (Figure 2c). By integrating these plots, we obtained the average charge, which was 5.698×10^{-4} C. The specific capacitance of $390 \mu\text{F}/\text{cm}^2$ was determined. These results indicate that the MXene/NF composite provides substantially higher specific capacitance than nickel foam alone, likely due to large electrochemical surface area and elevated capacitance of MXene.

Table 1. Comparison of electrocatalytic performance parameters using different electrode materials. The overpotential values are reported at a current density of $10 \text{ mA}/\text{cm}^2$, and Tafel slopes indicate the reaction kinetics for each electrode.

Parameters	MXene/NF (This work)	MXene@GO (This work)	Ni(OH) ₂	NiO-based
Overpotential	360 mV	290 mV	498 mV [18]	380 mV [19]
Tafel Slope	180 mV/dec	382 mV/dec	149 mV/dec [18]	299 mV/dec [19]

Table 1 shows that the MXene/NF electrode demonstrated superior electrochemical performance compared to Ni(OH)₂ and NiO-based electrodes. Balčiūnaitė A. et al. reported that Ni(OH)₂ exhibited an OER overpotential of 498 mV at $10 \text{ mA}/\text{cm}^2$ [18], whereas Rajneesh Kumar Mishra et al. showed that NiO-based electrodes had a lower OER overpotential of 380 mV [19]. In contrast, our MXene/NF electrode achieved a significantly lower OER overpotential of 360 mV, indicating enhanced catalytic activity. Moreover, our advanced MXene-GO-CB/NF electrode exhibited an even lower OER overpotential of 290 mV, further improving electrocatalytic performance.

Regarding reaction kinetics, Balčiūnaitė A. et al. reported that Ni(OH)₂ had a Tafel slope of 149 mV/dec for OER [18], whereas Rajneesh Kumar Mishra et al. showed that NiO had significantly higher values of 299 mV/dec (OER) [19]. Our MXene/NF electrode exhibited improved kinetics with Tafel slopes of 180 mV/dec (OER). Additionally, our MXene-GO-CB/NF electrode presented a Tafel slope of 382 mV/dec for OER, highlighting its different catalytic behavior.

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