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Multi-hetero-cation tuned electrocatalysts for efficient HER in pure saline water splitting

➤ Concept:

To enhance HER activity by engineering the active sites of MoS₂-based electrocatalysts through single- and multi-transition metal heteroatom doping at the cathode surface.

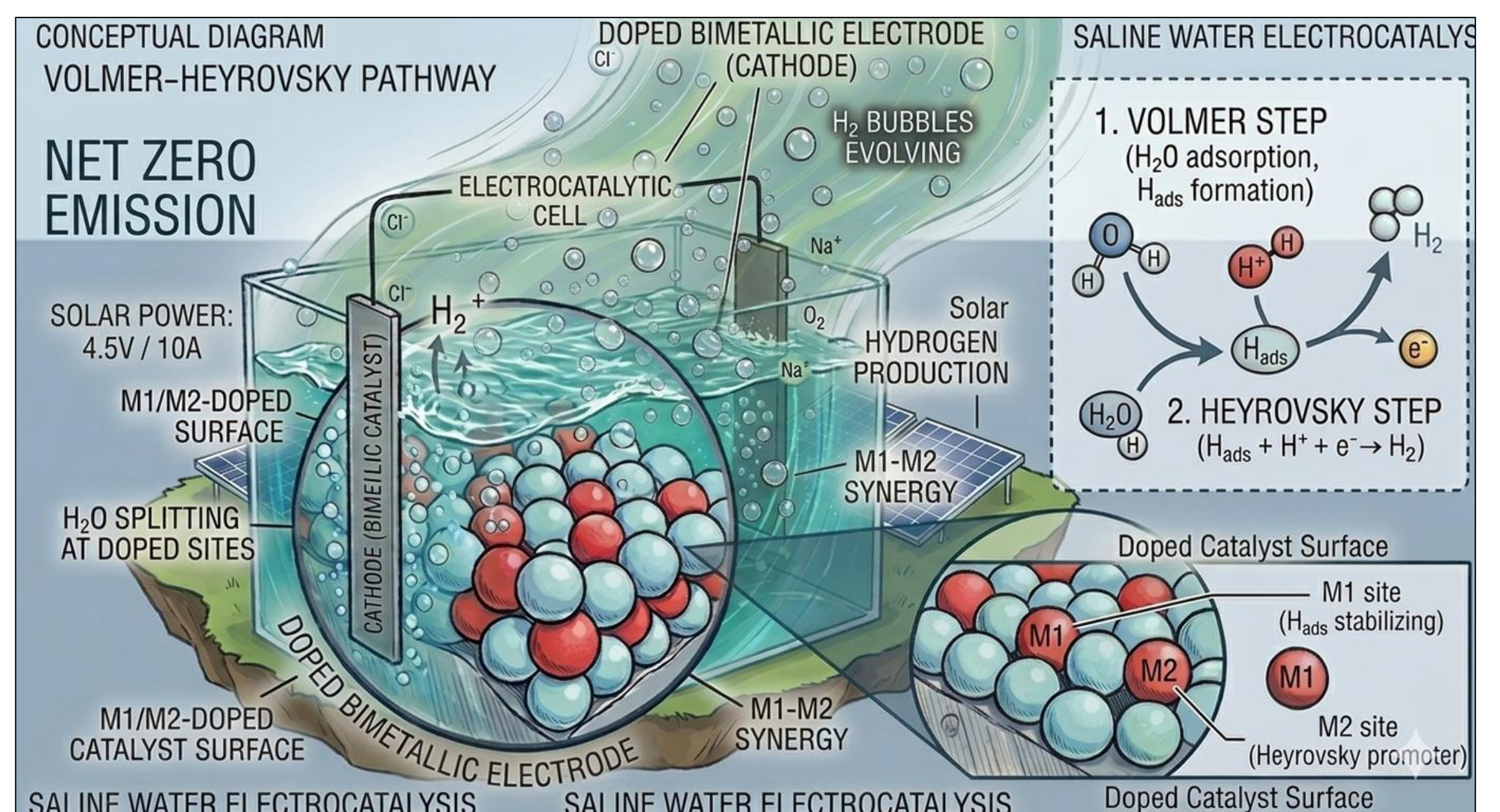
❖ Objectives:

- To reduce charge transfer resistance → enhanced charge mobility
- To increase double layer capacitance → increased ECSA

✓ Achieved:

Optimized electrocatalyst RuFeMoS₂

- Lower charge transfer resistance 5.24 Ω
- High double layer capacitance 11.2 μF
- Overpotential 340 mV at 10 mA
- Volmer-Heyrovsky kinetic pathway with the Tafel slope of 187 mV/dec



The authors acknowledge the use of Google Gemini (Google, LLC) for the generation of the conceptual diagram in the FIG 1. The authors reviewed and edited the output to ensure scientific accuracy and take full responsibility for the integrity of the final graphics.

Introduction

➤ Theoretical Hypothesis:

- ❑ HER Kinetic pathways at fixed external potential depends on charge mobility & availability of active sites on cathode surface
- ❑ Charge transfer resistance can be reduced by increasing number of electron donor cation sites

HER Kinetics in Alkaline Medium

Overall reaction: $2H_2O + 2e^- \rightarrow H_2 + 2OH^-$

Volmer step: $H_2O + e^- \rightarrow H^* + OH^-$ (adsorption)

Heyrovsky step: $H^* + H_2O + e^- \rightarrow H_2 + OH^-$ (electrochemical desorption)

Tafel step: $H^* + H^* \rightarrow H_2$ (recombination)

Analysis

Linear Sweep Voltammetry

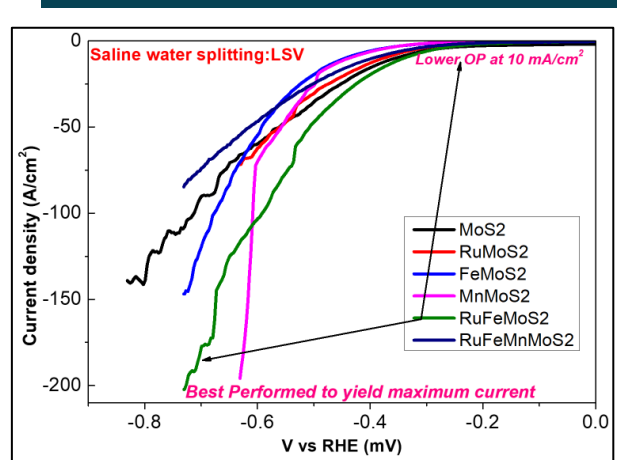
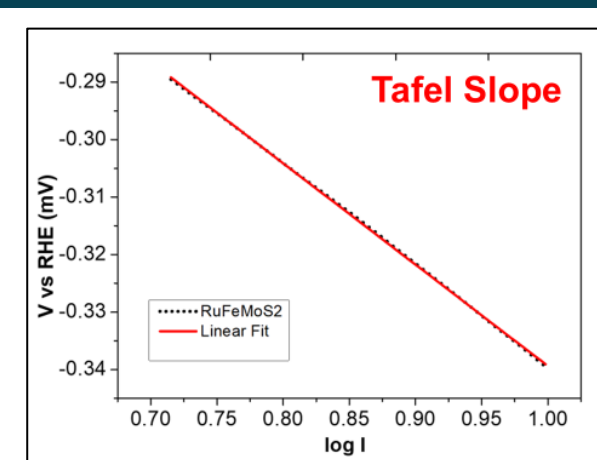


Fig 2-3: OP & Tafel slope of RuFeMoS₂ 340 mV, 187 mV/dec



Electrochemical Imp.

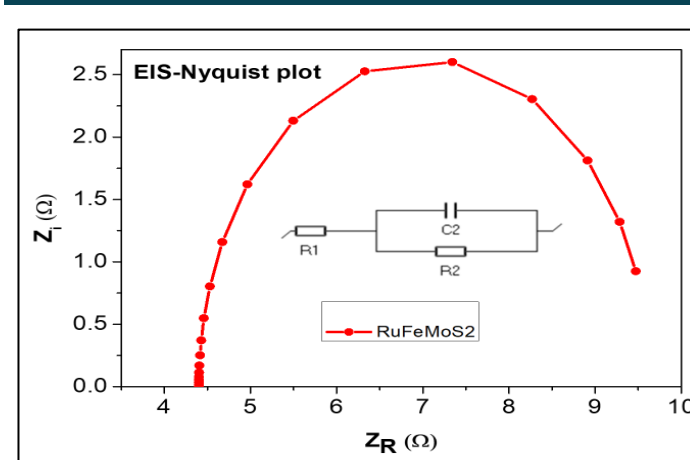
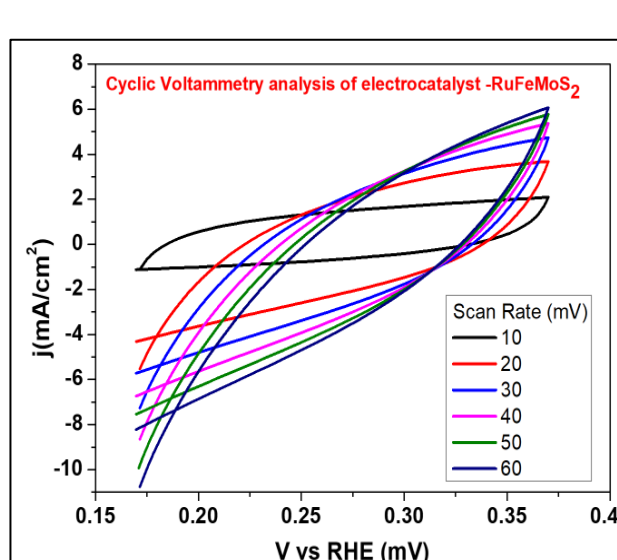
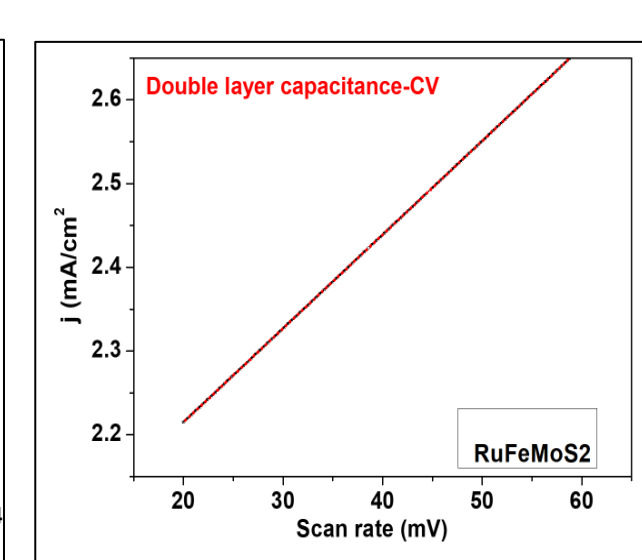


Fig 4: R_{ct} 5.24 Ω, fit circuit

Cyclic Voltammetry



Fi5 5-6: Calculation of double layer capacitance, linear fitting of $(J_{anode} - J_{cathode})/2$ with scan rate



❖ Electrochemical area = Cdl/Cs

Material Characteristics

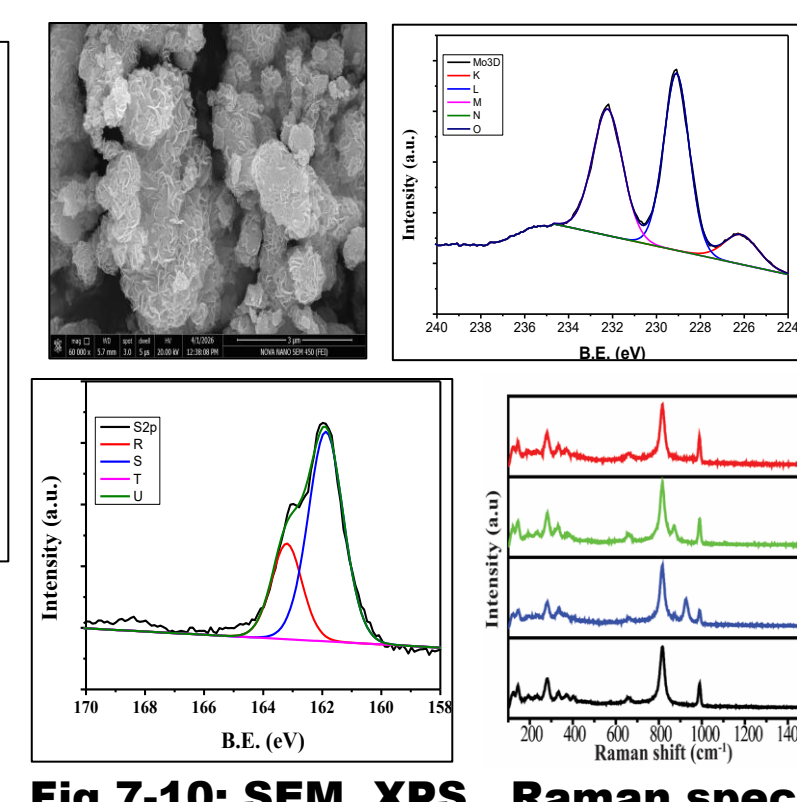


Fig 7-10: SEM, XPS, Raman spec

➤ Challenges:

- ❑ At cathode – HER: Cathode & catalyst material
- ❑ At anode – OER: competes with chlorine evolution
- ❑ Mass transport of ions through electrolyte
- ❑ Active sites blocking

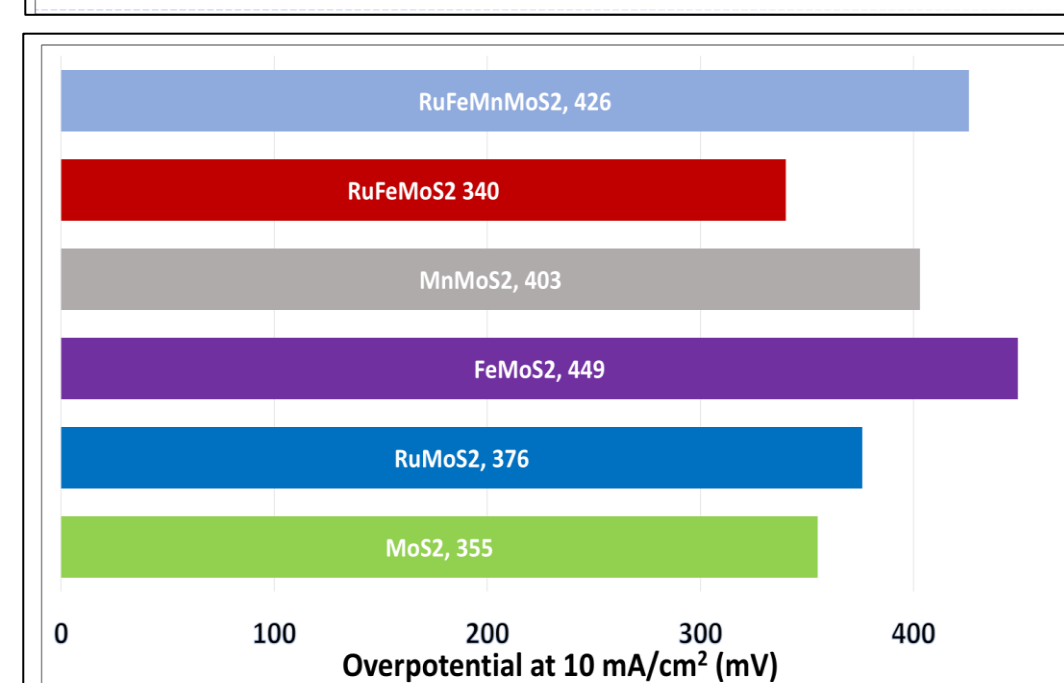
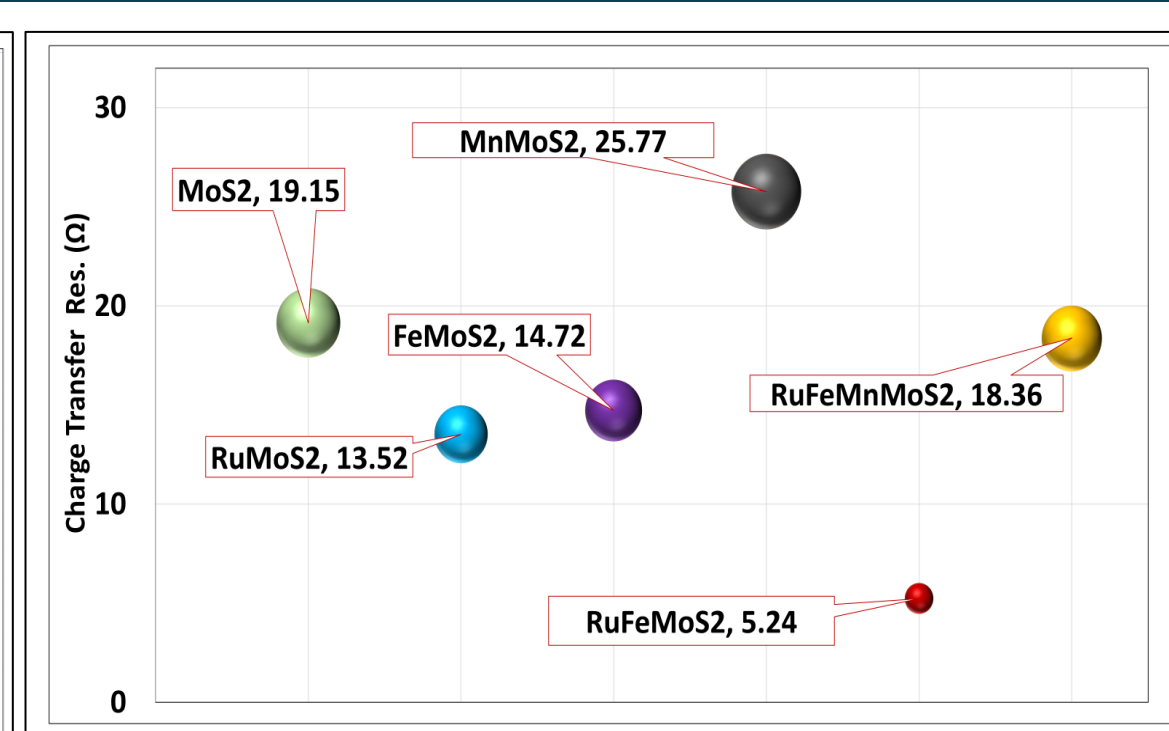
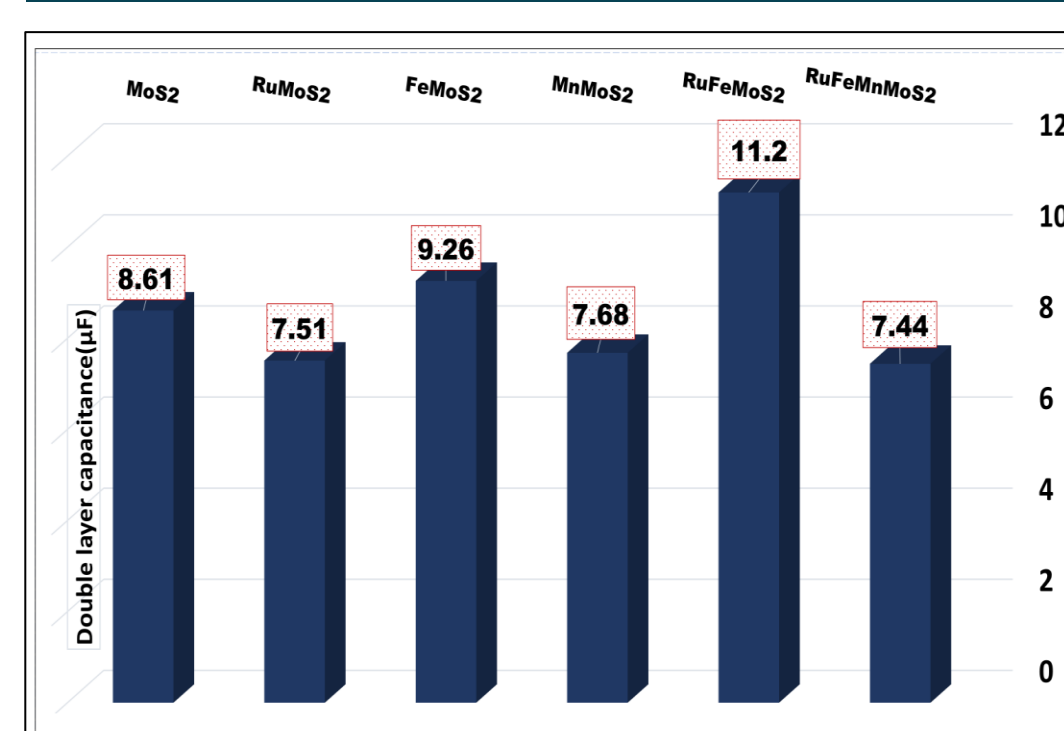
➤ Experimental Tuning

- ❑ Increasing number of active sites
- ❑ Increasing availability of electrons by doping with single/multi-hetero atoms of Fe, Mn, Ru on MoS₂

➤ Techniques:

- ❑ Hydrothermal synthesis
- ❑ Non-platinum electrodes – Ni, Graphite
- ❑ LSV for Overpotential, Tafel Slope
- ❑ CV for Double layer capacitance, ECSA
- ❑ EIS - Charge Transfer Resistance by Nyquist plot

Conclusions



- Promote net zero emission
- Route to green hydrogen
- Lower charge transfer resistance and double layer capacitance with RuFeMoS₂
- Use non-platinum electrodes such as Ni and graphite