Details of completed projects

1. Project details

a. *Title*: *Development of MXene-Hierarachical Transition Metal Suffide Hybrid Nanostructures as Electrocatalysts for Overall Water*

b. *Institute*: Pandit Deendayal Energy University Knowledge Corridor, Raisan Village, Gandhinagar – 382 426, Gujarat (State), INDIA

2. Aim / Objectives:

- Develop a room-temperature, HF-free molten-salt peroxidation method for synthesizing Ti_3C_2 MXene with improved safety and scalability.
- Investigate the structural/chemical evolution of Fe-replaced intermediate MXene (R-MXene) and its influence on functional terminations.
- Synthesize MoS_2/Ti_3C_2 MP-MXene hybrid structures using a one-step hydrothermal method and study their synergistic interaction.
- Evaluate HER activity of MP-MXene, R-MXene, HF-MXene, in situ HF-MXene, and MoS_2–MP-MXene using overpotential, Tafel slope, EIS, and ECSA.
- Optimize MoS_2–MP-MXene composition to maximize active sites and electron-transport pathways for advanced HER performance.

3. Executive Summary (*One page*):

The project aimed to develop efficient, scalable, and environmentally friendly electrocatalyst for hydrogen generation via water splitting. A novel HF-free MXene synthesis method was developed, resulting in enhanced safety and high yields. Using a molten-salt MAX peroxidation approach, $Ti_3C_2T_x$ MXene was functionalized for improved electron transfer, leading to enhance HER activity with overpotentials of 160 mV (10 mA/cm^2) and Tafel slopes of 48 mV/dec. Hydrothermal synthesis produced $MoS_2/Ti_3C_2T_x$ composites, which demonstrated superior catalytic performance (58 mV overpotential, 20 mV/dec Tafel slope). A MoS_2@Ti_3C_2 hybrid electrode was integrated into a custom-designed electrolyzer with an FAA-3-50 anion exchange membrane, enabling real-time hydrogen production. Hydrogen evolution was measured using the water displacement method, confirming scalable performance. This research establishes a sustainable pathway for hydrogen fuel production, combining green MXene synthesis, hybrid nanostructures, and effective electrode engineering.

4. Scope for further work

- Optimize MXene/MoS_2 ratios for improved dispersion and catalytic activity.
- Explore advanced slurry formulations and electrode deposition techniques.
- Enhance electrode–substrate interaction via surface modifications.
- Study electrocatalyst stabilization and activation methods for durability.
- Optimize gas separation and membrane design for hydrogen purity and efficiency.
- Conduct long-term durability tests and scale-up for practical applications.

5. Benefits visualized

- Efficient hydrogen production through water splitting.
- Enhanced catalytic activity and electron transfer.
- Cost-effective, scalable electrolyzer prototype.
- Improved electrolysis efficiency with selective ion transport.
- Contribution to sustainable clean energy technologies.