Modelling, control and optimization of high efficiency Hydrogen Evolution Reaction (HER) using MoTe2 as electrocatalyst

MOTIVATION

Climate change is one of the greatest challenges of the 21st century, and global Net Zero 2050 targets have identified green hydrogen as one of the pathways for achieving this goal because of its potential for carbon-free combustion with by-product of only water. Hydrogen is considered a very promising energy carrier as it contains nearly three times the energy content of gasoline per unit mass, is the simplest, lightest and most abundant chemical element in the universe.

Widespread hydrogen production is currently from fossil fuels and only a small proportion (circa 4%) is from water electrolysis powered by renewable energy, with the latter being fraught with problems of inefficiency, energy losses and high cost of noble metal catalysts.

As the catalytic splitting of water into its component hydrogen and oxygen is an energy intensive process, global research is currently focused on increasing cell efficiency, minimizing energy losses, development of alternative non-precious electrocatalysts to minimize initial capital costs and ensure long-term durability and performance of the equipment.

RESEARCH FOCUS

There are 5 main water electrolysis technologies available today with PEM being the most efficient:

- Alkaline Water Electrolysis (AWE)
- **Proton Exchange Membrane (PEM) Water Electrolysis – Fig 1**
- Anion Exchange Membrane (AEM) Water Electrolysis
- Solid Oxide Electrolysis Cell (SOEC)
- Proton Conducting Ceramic Electrolysers (PCCEL)

The research will focus on the design, modelling, and optimization of electrolytic cells for economical and efficient hydrogen production. The study aims to use computational tools such as Multiphysics modelling and machine learning to study, simulate and optimize the input, cell and output parameters that affect the cell efficiency.
Furthermore, Proton Exchange Membrane (**PEM**) electrolytic cells will be used as case study to analyse performance using non-precious electrocatalysts like MoTe2 in the Membrane Electrode Assembly (MEA).

METHODOLOGY

- Use computational tools and Multiphysics modelling such as COMSOL/ANSYS/MATLAB to capture the electrochemical and thermodynamic properties of the cells and predict polarization curves with changes in various input parameters.
- Carry out Hardware in the Loop (HIL) simulation and testing with real time data acquisition software and hardware on a pilot electrolytic cell to verify designed model.
- Carry out 3D printing using MoTe2 as catalyst in the Membrane Electrode Assembly (MEA) and test developed in-lab designs.
- Carry out machine learning using MATLAB/Python or other platform to capture sensor data, extract features, run models and prediction, optimize tune and deploy to simulation and pilot system.

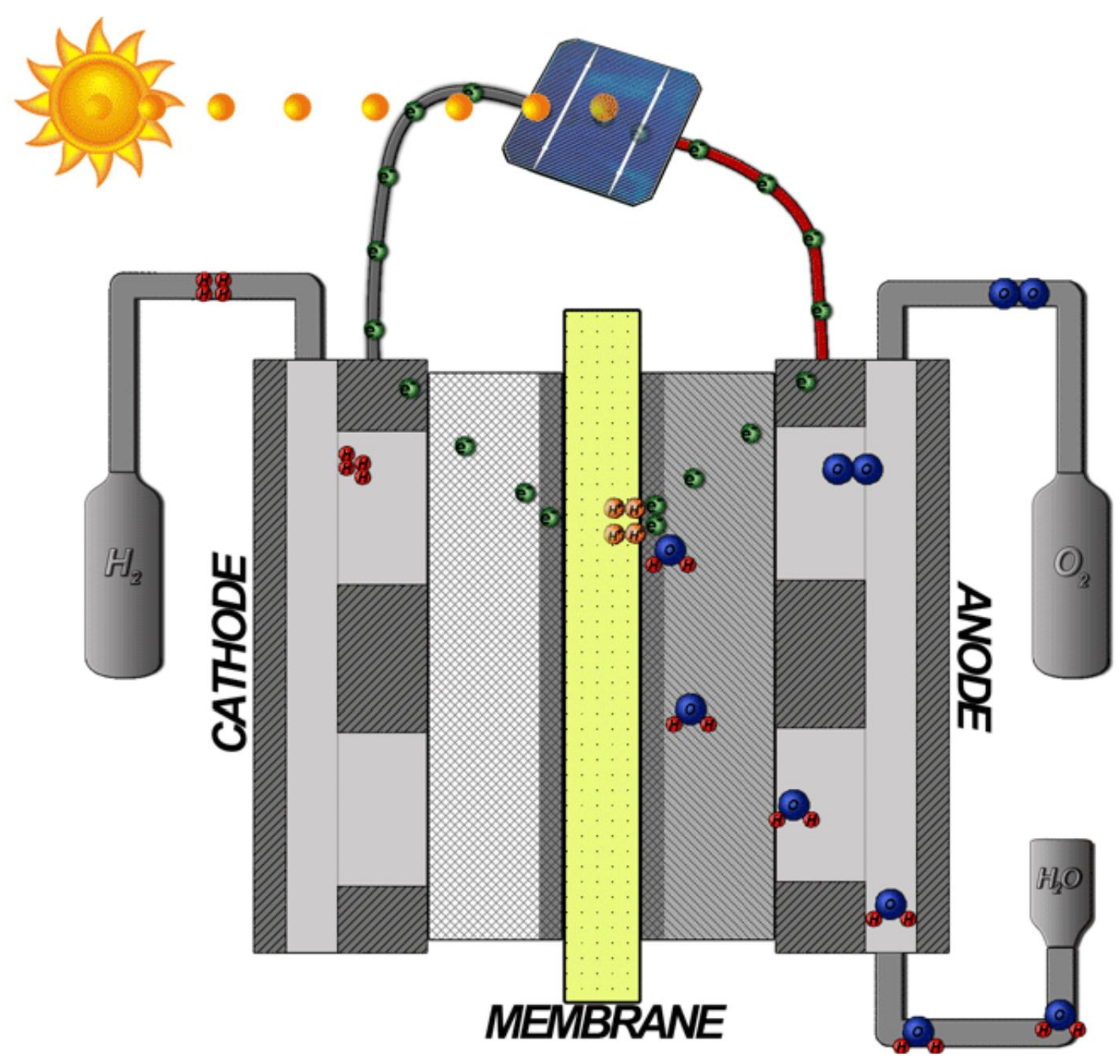

Figure 1: Solar-powered Proton Exchange Membrane **(PEM)** Electrolytic cell.

CONCLUSION & EXPECTED OUTCOMES

In conclusion, the project seeks to establish the relationship between operating parameters and cell efficiency. It aims to through cell design, parameter measurements, modelling and control optimization define a more efficient means of sustainable hydrogen production using MoTe2 as case-study electrocatalyst in a PEM electrolytic cell .

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