

# Chapter 1

## Introduction

### 1.1. Background and Motivation

The global shift toward sustainable and low-carbon energy systems has intensified the need for efficient, clean, and decentralized energy technologies. Conventional fossil fuel-based energy generation contributes significantly for greenhouse gas emissions, prompting a search for alternative solutions. Among the promising approaches, renewable energy sources such as solar photovoltaics (PV) and electro-chemical energy conversion technologies like fuel cells and electrolyzers have garnered significant attention. However, the intermittent nature of solar energy and the performance limitations of electrochemical systems present ongoing challenges.

Electrochemical systems, particularly those based on fuel cells and water electrolysis, are vital for future energy conversion and storage. The performance of these systems heavily depends on the efficiency of electrode reactions, notably the oxygen evolution reaction (OER) and methanol oxidation reaction (MOR). The development of cost-effective and high-performance electrocatalysts for these reactions is crucial for advancing hydrogen production and fuel cell technologies.

Simultaneously, solar PV systems have become increasingly viable due to technological advances and cost reductions. Optimizing the engineering aspects of PV systems, including component selection, layout design, performance modelling, and integration strategies, is essential to maximize energy yield and reliability. There is a growing interest

in hybrid electrical systems that integrate solar PV with fuel cells or electrolyzers to ensure continuous and clean power supply.

This doctoral research addresses two distinct but complementary areas: the development of efficient anode electrocatalysts as electrode materials for Oxygen Evolution Reaction (OER) and Methanol Oxidation Reaction (MOR) and the engineering and performance analysis of solar photovoltaic power systems. Early onset potentials with efficient electrode materials for OER on anodic side of the cell, reduces the amount of input potentials for hydrogen generation (Ideal 1.23V Vs RHE). On similar lines, these electrode materials were employed for Direct Methanol fuel cell, where in reduced voltages on anodic side indicates the reduced losses in the Methanol fuel cell output, thus a way forward for efficiency enhancement. Together, these contributions aim to support the development of advanced hybrid electrical systems for sustainable energy applications.

## **1.2. Overview**

This work spans both materials-level and system-level investigations. The material development research focuses on transition metal-based electrocatalysts developed via techniques such as Melt spinning and surface modification techniques like anodization, cathodic corrosion and de-alloying. The performance metrics include over potential's, current density, charge transfer resistance, Tafel characteristics, and long-term durability under Oxygen evolution reaction (OER) and Methanol oxidation reaction (MOR) conditions towards Hydrogen generation at cathode and reduced internal voltage losses in Direct methanol fuel cell respectively.

The system-level study involves the engineering of solar PV power plants, including component sizing, layout optimization, and yield analysis using simulation tools. Though

the two areas are treated as parallel themes, their relevance to hybrid energy systems forms a common thread.

### 1.3. Key Challenges and Constraints

Several challenges and constraints were encountered during the course of this research:

- **Material limitations:** Achieving high electrocatalytic activity and stability using earth-abundant, low-cost materials for OER and MOR remains difficult. Controlling surface structure, composition, and conductivity is critical and technically demanding.
- **Scalability:** Translating lab-scale catalyst synthesis methods into scalable and reproducible procedures is a major hurdle for practical applications.
- **Electrochemical characterization:** Accurately assessing catalyst performance involves advanced techniques that require careful calibration and interpretation, especially under simulated real-world conditions.
- **Solar PV system optimization:** Designing PV systems tailored to specific load profiles and environmental conditions involves multiple variables, including irradiance patterns, tilt angles, inverter efficiency, and shading effects.
- **System integration:** Exploring the interoperability of solar PV and electrochemical systems within a hybrid electrical framework presents both control and operational complexity.

Overcoming these constraints requires an interdisciplinary approach, combining materials science, Electrochemistry, Energy systems engineering and Electrical Engineering.

## 1.4 Research Objectives and Scope of Work

### ◆ 1. Research Objectives

The primary goal of this research is to address challenges in energy generation by investigating novel materials for electrochemical reactions and exploring efficient system-level integration strategies. The research is anchored on the development of Efficient electrode materials for Hydrogen generation, Methanol Fuel cell and design cum development solar photovoltaic (PV) systems, a way towards the hybrid electrical systems.

#### The key objectives are:

- To Synthesize and Develop Novel Electrocatalyst materials capable of enhancing performance in:
  - Oxygen Evolution Reaction (OER) for water splitting and Hydrogen generation towards the Cathodic side.
  - Methanol Oxidation Reaction (MOR) for direct methanol fuel cell DMFC applications.
- To Characterize and Evaluate the Developed Materials using advanced techniques to evaluate:
  - Crystallographic, morphological, and surface properties.
  - Electrochemical performance and stability for OER/MOR.
- To Design and simulate a grid-connected solar PV system, optimized for real-site conditions, focusing on:

- Load analysis, PV sizing, component selection.
- Performance modelling using tools like PV-syst.
- To perform techno-economic and environmental analysis of the PV plant in comparison to standalone setups.

## ◆ 2. Scope of the work

This interdisciplinary research spans both Material development and System level engineering. The scope is structured in two complementary layers:

### A. Materials Level (Electro-catalyst):

- Focused on catalyst design for enhanced electrochemical energy conversion.
- Covers non-precious metal-based catalysts for sustainability and cost-effectiveness.
- Electrochemical evaluation under alkaline conditions relevant to practical fuel cells or electrolyzers.
- Lab-scale proof of concept validating OER/MOR activity and stability.

### B. System-Level (Solar PV):

- Realistic design of a solar PV system including irradiation, load profile, and component specifications.
- Use of Hardware and simulation platforms to predict energy output, performance ratio, and reliability.
- Emphasis on energy optimization, load balancing, and backup strategies.

Summarised objectives of the study is as follows:

- To develop and characterize efficient, low-cost anode electrocatalysts for the oxygen evolution reaction (OER) and methanol oxidation reaction (MOR).
- To investigate the electrochemical performance, stability, and surface properties of the developed catalysts using advanced characterization techniques.
- To design, simulate, and evaluate the performance of solar photovoltaic power systems with emphasis on engineering optimization.
- To explore the integration potential of electrochemical and photovoltaic systems within a hybrid electrical framework.

**Limitations Acknowledged:**

- Catalyst testing is limited to laboratory-scale electrochemical cells and not full-stack DMFC or water electrolyzer prototypes as it needs full-fledged infrastructure.
- Experimental testing of full hybrid system integration (PV + fuel cell) is not possible due to infrastructure constraints and left for future scope of work, by using different types of Electrode materials.

## 1.5. Detailed Methodology

### Part A: Electro-catalyst Development for OER/MOR

#### 1. Materials Synthesis and Preparation

Selection of catalyst Material: Transition metal-based compounds such as Ni, Co, Fe oxides, and phosphides were selected due to their promising activity toward OER and MOR reactions.

- Material preparation Methods:
  - Amorphous Electrical steel ribbons developed through melt-spinning.
  - Surface modifications.
  - De-alloying.

#### 2. Characterization of Electrode Material (Catalysts)

- Structural Characterization:
  - X-ray Diffraction (XRD) to confirm phase purity and crystallinity.
  - Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) to analyse morphology and nanostructure.
- Surface and Elemental Analysis:
  - X-ray Photoelectron Spectroscopy (XPS) for surface oxidation states.
  - Energy-Dispersive X-ray Spectroscopy (EDS) for elemental distribution.
- Surface Area & Porosity:

- 3-D profilometry analysis to determine surface profiling.

### 3. Electrochemical Testing

- Electrode Fabrication:
  - The catalyst was drop-casted or spray-coated on glassy carbon electrode (GCE) or nickel foam substrate.
- Electrochemical Setup:
  - A standard three-electrode system with Ag/AgCl reference, platinum counter electrode, and working electrode.
  - Experiments were conducted in 1.0 M KOH or NaOH electrolyte.
- Measurements:
  - Linear Sweep Voltammetry (LSV) to determine over-potential and onset potential.
  - Tafel slope analysis to understand reaction kinetics.
  - Electrochemical Impedance Spectroscopy (EIS) to assess charge transfer resistance.
  - Chronoamperometry for stability and durability testing.
- Comparative Study:
  - Performance was benchmarked against standard commercial catalysts like RuO<sub>2</sub> or Pt/C.

**Part B: Solar PV Plant Engineering****1. Site Selection and Load Analysis**

- Selection of industrial or academic campus location for practical deployment.
- Load assessment was carried out for daily, monthly energy consumption patterns.
- Consideration of seasonal variability and peak demand.

**2. Solar Resource Assessment**

- Solar irradiance data was collected using PVsyst and on-site pyrometers.
- Tilt angle optimization and shadow analysis conducted using simulation tools.

**3. System Design**

- **PV Array Sizing:**
  - Based on peak load and energy demand.
  - Integration of battery storage for hybrid operation considered.
- **Component Selection:**
  - Selection of panels (mono/poly crystalline), inverters, mounting structures, MPPT systems.
- **Wiring, Safety & Protections:**
  - Fuse ratings, grounding, surge protection, and circuit breakers based on IS/IEC standards.

**4. Simulation & Performance Modelling**

- **Software Used:**

- PVsyst was used to simulate energy output and design simulations.
- **Performance Metrics:**
  - Capacity Utilization Factor (CUF), Performance Ratio (PR), and specific yield were analyzed.

## 5. Economic and Environmental Assessment

- Levelized Cost of Energy (LCOE) calculations.
- Payback period and ROI analyses.
- Life cycle assessment from solar system vs other Renewable and Non-renewable sources.

The above methodology ensured a holistic approach covering both material-level catalyst innovations and system-level PV plant design. The dual investigation enabled validation of catalyst performance in laboratory conditions and relevance in broader renewable energy integration strategies.

## 1.6. Thesis Organization

The thesis is organized into the following chapters:

- Chapter 1 provides an introduction to the research problem, objectives, and scope.
- Chapter 2 reviews relevant literature on Water catalysis, Hydrogen generation, OER electro-catalysis, fuel cells, and photovoltaic engineering.
- Chapter 3 presents the experimental details and methodologies used to prepare the catalysts, evaluate the electro-chemical performance of the catalyst and material characterisation tools used in the thesis.

- Chapter 4 details the nano-crystallization of Nickel oxo/hydroxo complex on (NiFeCr)SiB amorphous ribbon through cathodic corrosion technique for Alkaline Oxygen evolution reaction and Methanol oxidation reaction.
- Chapter 5 details the Self-Supported De-Alloyed Nickel-Amorphous Ribbons used for enhanced electro-catalysis, including OER and MOR.
- Chapter 6 covers the comprehensive plant design Aspects and Performance assessment of On grid solar 500 kWp solar PV plant which includes, detailed engineering design, simulation, and performance evaluation of PV system.
- Chapter 7 includes the Techno-economics and Environmental impact assessment of 500 kWp On-grid rooftop PV plant using the real time field data and with Life cycle assessment software tools.

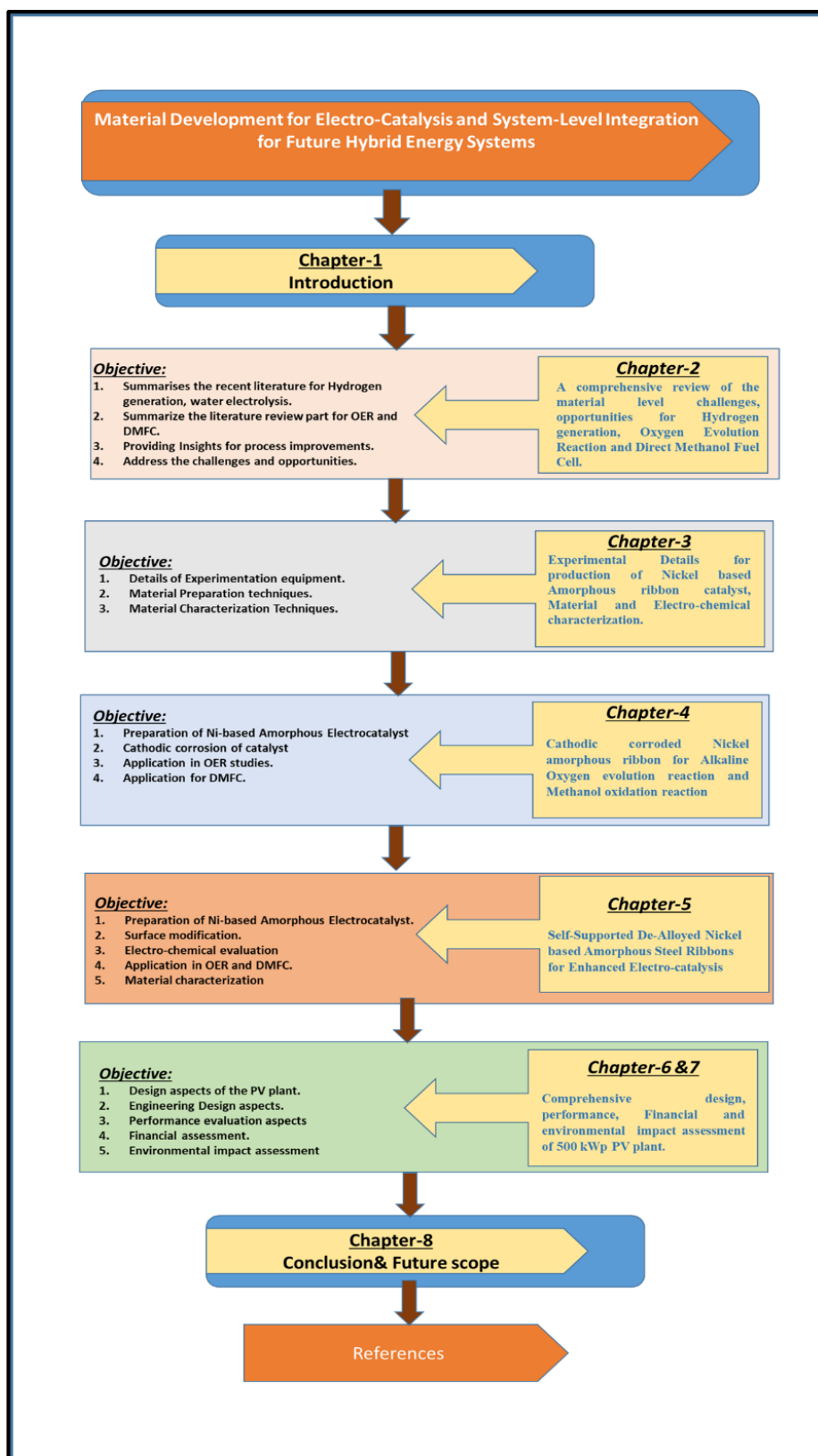


Figure 1.1- Brief thesis outline