

Preface

Over the past few decades, scientists and climate activists have paid close attention to energy conversion, storage, and environmental protection issues. The continual and ever-increasing consumption of fossil fuels results in a slew of critical issues, including severe environmental contamination and a near-term lack of conventional fossil fuels. To overcome these serious issues, we must introduce a renewable and clean energy system alternative to solve existing environmental pollution problems while addressing energy shortage problems. For this reason, countries worldwide have invested considerable effort toward producing and storing renewable and carbon-free energy sources such as tidal, wind, geothermal, hydroelectric, and solar. Despite their merits of being environmentally friendly, intermittent nature due to weather and time-dependent, low energy delivery efficiency, location specificity, and expensive maintenance limits their uses globally. Therefore, the need for effective and affordable energy conversion and storage technologies, including the synthesis of novel materials and effective processing methods, is highly urgent. The United Nations General Assembly's 2015 Sustainable Development Goals (SDGs) 6, 7, and 14 also include these criteria.

Hydrogen (H₂) is a good candidate for energy carriers in fuel cells due to its unique advantages of maximum energy density (120-140 MJ kg⁻¹) with carbon-free features, making it a suitable candidate for changing the global energy structure demand in the future. It can be used as a fuel to replace traditional fossil fuels and stored as extra energy using a system that interfaces with the renewable energy system for electricity. Hence, environmentally friendly and highly efficient techniques are required to produce clean and cost-effective hydrogens. In this regard, electrochemical water splitting techniques are the most promising approaches, as they rely on unrestricted water sources with a massive high-purity H₂ production capability, higher flexibility, and production efficiency. Noble metal Pt is the best electrocatalyst for

electrocatalytic H₂ production with high current density and lower Tafel slope value, but the exorbitant price limits its use for commercial purposes. The research communities are paying much attention to an alternative to the precious noble metal. In this regard, composites of conjugated polymer with transition metal compounds as electrocatalysts and electrode materials for energy storage are of great interest. These materials have the merits of being low-cost, earth-abundant, noble metal-free, and environmentally friendly with very high electrochemical performance.

Conjugated polymer-based (specially N-containing) nanocomposites with metals, bimetals, and their compounds emerged as promising candidates for electrocatalysis and electrode materials for energy storage in recent years due to the vibrant superiority of compositional and morphological flexibilities, easy synthesis, and tunable diversity. Conducting polymer-based composite materials also has advantages concerning their cost-effectiveness, processability, and environmentally friendly and nontoxic nature.

The present thesis aims to investigate the electrocatalytic and electrochemical charge storage properties of conjugated polymer-based composites to address energy problems and better environmental protection. We have focused on synthesizing novel composites via the functionalization of conjugated polymer with transition metal oxides and NASICON-structured materials that result in many-fold enhancements in the electrochemical performance due to synergism.

The present thesis work is divided into seven chapters. *Chapter 1* deals with conjugated polymer, its historical background, classification, origin and mechanism of conductivity, properties, applications and limitations. This chapter also deals with the composites of the conjugated polymer, various techniques for composite formation, their improved properties and multiple applications. This chapter also discusses conjugated polymer composites'

electrocatalytic and charge storage properties. This chapter also discusses the basic principle and mechanism of electrocatalysis (FA oxidation and HER) and charge storage and their various important parameters. **Chapter 2** briefly details the different tools and instruments used for characterizing the as-synthesized composite materials and electrochemical tools and terminology for application purposes. **Chapter 3** discusses the electro-oxidation of formic acid properties of polycarbazole/ WO_3 composites (PCz/WO_3) prepared using various weight % of WO_3 incorporated into the fixed PCz matrix at the monomeric level. This investigation sheds light on exploring low-cost, environmentally friendly electrocatalysts with high performance as an alternative for noble metals. **Chapter 4** deals with the HER properties of nanocomposites of polypyrrole and NASICON-structured NFS (PPy/NFS) synthesized using various weight % of NFS immobilized into a fixed amount of PPy matrix at the monomeric level. The optimized PPy/NFS composites ratio offers high catalytic activity and stability towards HER. **Chapter 5** further explores the enhanced catalytic activity towards HER of PPy/Ni -doped NFS composites via incorporating a varying amount of Ni doping into the NFS. The obtained results significantly highlight the role of Ni doping in NFS for enhancing the active sites and ease of charge transfer as well as ease of hydrogen adsorption resulting in excellent HER activity by $\text{PPy}/\text{NFS}(\text{Ni})$ composites. The improved HER catalytic activity of $\text{PPy}/\text{NFS}(\text{Ni})$ composites is comparable to that of noble metal Pt. It can be treated as an alternative to the costly noble metal Pt catalyst for HER. **Chapter 6** deals with the charge storage property of PPy/NFS and PPy/Ni -doped NFS composites as a supercapacitor. The electrochemical results show that the composites have good charge storage capacity and can be a promising candidate for supercapacitor application. **Chapter 7** summarizes the complete research work during the Ph.D. and also discusses the future scope of work.

The present thesis has compiled all the published data in *ACS Energy & Fuel* (2022 IF: 4.654), and *Materials Chemistry and Physics* (2022 IF: 4.778).