Chapter 6

Conclusion

&

Future Scope

6.1 Conclusion

Hydrogen is a unique molecule that has the potency to revolutionize the era of global energy consumption by substituting methane most commonly known as Natural gas. Electrocatalytic hydrogen production method is the most efficient method both in terms of its viable implication as well as the green production procedure. Unfortunately, there are numerous challenges that hold back the widespread commercialization of the process. In this thesis, we have primarily tried to address several key research challenges like the catalyst material derived from the alternative of the noble metals, stability, corrosion resistivity of the catalyst in the acidic medium as well as the mass and charge transport properties to make electrocatalytic hydrogen evolution reaction a practical solution. Also, we have adopted very simple catalyst preparation strategies like solvothermal, *in situ* sol-gel method, *in situ* polymerization method, and pyrolysis method for our catalyst preparation. All these catalysts are proven to be efficient and stable HER electrocatalysts. We have also elaborately discussed the supercapacitor property of our synthesized material along with its electrocatalytic property towards HER in one of the chapters. Our research findings conclude that the synergistic effect arising from integrating different components increases the intrinsic activity of the composite by increasing number of active sites, and overall electrical conductivity. The major outcomes of our studies are summarized below:

1. Modulation of electronic density states of carbon in Expanded Graphite by multifaceted Cu doped Co_2P particle for electrocatalytic hydrogen evolution reaction in aqueous acidic medium.

- Cu doped Co_2P@EG exhibits optimum catalytic activity with 0.005 wt% of Cu content, The electrocatalyst delivers HER with an overpotential value of 81 mV (η_{10}) which has proved it to be a potential Pt free electrocatalytic material for HER.
- Density Functional Theory (DFT) affirms that upon incorporation of Cu-doped Co_2P particle in expanded graphite the electronic density of the carbon atom gets facilitated to carry out HER efficiently.

2. Iron-doped titania/multiwalled carbon nanotube nanocomposite as a robust electrocatalyst for hydrogen evolution reaction in aqueous acidic medium.

- Fe doped TiO_2/MWCNT has exhibited the best catalytic activity towards HER with 0.50 wt% of MWCNT content. The oxide-based catalyst requires an overpotential value of 0.221 V (η_{10}) vs RHE.
- The electrocatalyst exhibits good stability in acidic medium.

3. Iron doped titania/ Polyaniline composite as an efficient electrocatalyst for hydrogen evolution reaction in acidic medium.

- The Fe doped TiO_2/PANI has been synthesized by an easy in situ chemical oxidative polymerization of aniline in presence of Fe doped TiO_2.
- The activity of the synthesized catalyst towards HER was maximum with 0.45 wt% of PANI which requires an overpotential value of 0.285 V (η_{10}) vs RHE.

4. Bi-functional hierarchically porous N, P co-doped reduced graphene oxide aerogel as a symmetric supercapacitor material and a robust hydrogen evolution reaction electrocatalyst.

- N, P co-doped reduced graphene oxide aerogel acts as an efficient metal free electrocatalyst towards HER with an overpotential value of 0.351 V at a current density of 10 mA cm^{-2}.
- The supercapacitor works within a wide range of potential window of 2 V and delivers energy density of 84 W h kg^{-1} capacitance retention 92%.

6.2 Future scope:

We have carried out a limited study and focused mainly on the study of electrochemical behaviour of the catalysts towards HER. Despite high efficiency of these catalysts in HER further advancements are necessary. Keeping that in mind, future work could be focused on:

(i) Further Optimization in the synthesis procedures can be done by changing the aspect ratios of the components in the metal clusters, integrating the metal-based electrocatalyst with other conductive carbon-based nanomaterials, etc.

(ii) These active nanomaterials could be explored in other energy-related applications like methanol fuel cell, oxygen reduction reaction (ORR), etc.