$MoSe_2$ Nanostructures Based Electrocatalysts for Electrolyzer and Zinc-air Battery

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By

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Chapter 7 Conclusion and Future Scope of The Work

7.1 Conclusion

In conclusion, the present thesis work is mainly focused on the synthesis of different materials such as pristine $MoSe_2$ nanosheets, in-situ grown $MoSe_2$ nanostructures over different conducting substrate ($MoSe_2$-CCP and $MoSe_2$-Ni foam), Bimetal oxides ($CoFe_2O_4$, $NiFe_2O_4$ and $NiCo_2O_4$/NiO), Bimetal oxide- $MoSe_2$ hybrid nanostructures ($CoFe_2O_4$-$MoSe_2$, $NiFe_2O_4$-$MoSe_2$ and $NiCo_2O_4$/NiO-$MoSe_2$) and Ni decorated $MoSe_2$ nanocomposites via hydrothermal technique for hydrogen evolution reaction (HER), oxygen evolution reaction (OER), electrolyzer and zinc air battery applications. Different characterization techniques such as SEM, TEM, XRD, XPS, Raman and FTIR spectroscopy have been used to characterize the prepared materials. Different electrochemical measurement methods like CV, LSV, EIS and chronoamperometry techniques have been utilized to evaluate HER and OER activities. In case of electrolyzer application, we have successfully demonstrated real time hydrogen and oxygen generation using a prototype electrochemical cell in 1M KOH using binder free $MoSe_2$ electrodes and Ni-$MoSe_2$ nanocomposites based electrodes. In case of zinc air battery application, we have demonstrated the battery performance of pristine $MoSe_2$ and bimetal oxides-$MoSe_2$-hybrid nanostructures as air cathode in high alkaline (6M KOH + 0.2 M zinc acetate) electrolyte. Different battery measurements like open circuit potential, specific capacity, galvanodynamic and galvanostatic charge-discharge measurements have been performed to evaluate the battery performance.

Important Finding of The Present Work

- In the present work, we have successfully demonstrated HER activity of binder free electrode ($MoSe_2$-CCP and $MoSe_2$-Ni foam) and different Ni-$MoSe_2$ nanocomposites.

In case of binder free electrodes, $MoSe_2$-Ni foam shows η_{10} ~100 mV and Tafel slope ~73 mV dec^{-1} in 1M KOH for HER, while in 0.5M H_2SO_4, $MoSe_2$-CCP electrodes displays η_{10}~ 143 mV and Tafel's slope ~53 mV dec^{-1}. The better performance of binder-free $MoSe_2$-Ni foam electrode in 1M KOH is attributed to better conductivity of Ni substrate and wrinkled vertical structure of $MoSe_2$. Better performance of $MoSe_2$-CCP electrode in 0.5M H_2SO_4 can be attributed to stable nature of CCP in acidic environment. The wrinkled vertical structure of $MoSe_2$ in binder free electrodes provides higher number of exposed edges and reduces charge transfer resistance for better electrocatalytic activity. Among different Ni-$MoSe_2$ nanocomposites (5%, 10% and 20%), Ni-$MoSe_2$ (10%) shows lowest η_{10} ~141 mV and Tafel slope ~60 mV dec^{-1} for HER activity. The higher HER activity of Ni-$MoSe_2$ (10%) is due to the optimum presence of Ni atoms over $MoSe_2$, which provides a high synergistic effect between $MoSe_2$ and Ni nanoparticle.

- ❖ We have also successfully demonstrated the OER activity of binder free electrodes ($MoSe_2$-CCP and $MoSe_2$-Ni foam), bimetal oxides, bimetal oxide-$MoSe_2$ hybrid nanostructure and Ni-$MoSe_2$ nanocomposites based electrodes in alkaline medium. In case of binder free electrodes, $MoSe_2$-Ni foam shows excellent OER performance (η_{50} ~292 mV and Tafel' slope ~20 mV dec^{-1}) due to wrinkled vertical structure of $MoSe_2$ and better conductivity of Ni substrate. Among Ni-$MoSe_2$ nanocomposites, $MoSe_2$-Ni (10%) shows best OER activity with η_{10} ~277 mV and Tafel slope ~53 mV dec^{-1} compared to Ni-$MoSe_2$ (20%) (η_{10} ~ 293 mV, Tafel slope ~57 mV dec^{-1}), Ni-$MoSe_2$ (5%) (η_{10} ~ 306 mV, Tafel slope ~ 66 mV dec^{-1}) due to the optimum and uniform distribution of Ni atoms over $MoSe_2$ in 10% nanocomposite, which provides a high synergistic effect between $MoSe_2$ and Ni. Among bimetal oxide-$MoSe_2$ hybrid nanostructures, $NiFe_2O_4$-$MoSe_2$ shows best OER activity (η_{10} ~ 218 mV and Tafel slope

~37 mV dec^{-1}) due to the synergistic effect between $MoSe_2$ and $NiFe_2O_4$, which enhances the conductivity, oxygen mobility, and active sites of the catalysts.

- ❖ Further, we have successfully analyzed the performance of designed alkaline water electrolyzer using binder-free electrodes ($MoSe_2$-CCP and $MoSe_2$-Ni foam), and Ni-$MoSe_2$ nanocomposites based electrodes. The $MoSe_2$-Ni foam based electrolyzer shows a overpotential of 335 mV at a current density of 10 mA cm^{-2} with 96% faradaic efficiency for H_2 and O_2, due to its better HER and OER activities. Among Ni-$MoSe_2$ nanocomposites, Ni-$MoSe_2$ (10%) shows overpotential of 284 mV at a current density of 10 mA cm^{-2} with 93% faradaic efficiency for H_2 and O_2 attributed to synergistic effect between $MoSe_2$ and Ni nanoparticle in Ni-$MoSe_2$ nanocomposites.
- ❖ Further, we have also successfully designed and tested Zinc air batteries with pristine $MoSe_2$ nanosheets and its hybrid nanostructures with bimetal oxides ($CoFe_2O_4$, $NiCo_2O_4$/NiO, and $NiFe_2O_4$) as air cathodes in 6M KOH + 0.2 M zinc acetate electrolyte. Among studied battery, the $NiFe_2O_4$-$MoSe_2$ shows the best performance, with an open-circuit voltage of 1.43 V, a specific capacity of 1025 mA h g_{Zn}^{-1}, an energy density of 1204 W h kg_{Zn}^{-1}, and a high-power density of 176 mW cm^{-2}. The $NiFe_2O_4$-$MoSe_2$ based Zn-air battery also demonstrates excellent stability and durability for 24 hours of continuous charge-discharge cycles. High performance of $NiFe_2O_4$-$MoSe_2$ hybrid nanostructure is due to the synergistic effect between $MoSe_2$ and $NiFe_2O_4$, which enhances the conductivity, oxygen mobility, and active sites of the catalysts.

7.2 Future scope of the work

- ❖ In future, hydrothermal synthesis route can be explored to synthesize different morphologies of $MoSe_2$ nanostructures and heterostructure with other transition metal dichalcogenide (TMDCs) materials.

- In future, new synthesis methods can be elucidated to synthesize in-situ grown $MoSe_2$ of different morphology on different substrates.
- The HER and OER activity of synthesized materials can be explored in different electrolyzer.
- Solid electrolyte based electrolyzer and zinc air battery can be explored using $MoSe_2$ based nanomaterials as electrocatalyst. This may lead to the development of flexible energy storage devices.