

## **Project goal**

The aim of this project is to develop  $\text{Fe}_x\text{M}_{1-x}\text{S}$  ( $\text{M}=\text{W}, \text{Ni}, \text{Co}, \text{Mo}$ ) and  $\text{FeM}_2\text{S}_4$  ( $\text{M}=\text{Co}, \text{Ni}, \text{Mo}, \text{W}$ ) nanoparticles on the surface of  $\text{NiCo}_2\text{Se}_4$  as excellent electrocatalysts for overall water splitting in order to replace precious metals.

## **Significance of project**

Hydrogen is considered as auspicious energy carrier due to their high energy density, renewability, and zero carbon emission. Electrocatalytic overall water splitting is the most reliable technology for pure hydrogen production from cheap source of water. Highly efficient and cheap electrocatalyst is supreme desire for overall water splitting. Among different available electrocatalysts, transition metal chalcogenides have attracted an extensive research attention due to their low cost, high availability, environment friendliness and excellent response to overall water splitting. In addition, hetero-structure gained special research attention as the interface at hetero-structure may facilitate charge movement between their components, enhanced intrinsic activity, tune the binding affinity for reaction intermediate and their synergism boost reaction kinetics. We have planned to design  $\text{Fe}_x\text{M}_{1-x}\text{S}$  ( $\text{M}=\text{W}, \text{Ni}, \text{Co}, \text{Mo}$ ) and  $\text{FeM}_2\text{S}_4$  ( $\text{M}=\text{Co}, \text{Ni}, \text{Mo}, \text{W}$ ) nanoparticles with different morphologies. These materials will be decorated on the surface of  $\text{NiCo}_2\text{Se}_4$  nanoflowers to avoid the agglomeration of chalcogenides nanomaterials, utilize the benefits of heteroatom, multi-transition atom and their synergism. In addition, Se is highly active towards oxygen evolution reaction which will be further boosted by Ni and Co. The interaction of heteroatom, modified and high electronic cloud and synergism of metals will facilitate the transport of electron and oxygen evolution reaction which exhibits sluggish kinetics during overall water splitting. Furthermore, it is well-known that bi-metals are better in performance than mono-metal, so multi-metals will of course boost their electrochemical application for overall water splitting.

## **Expected results**

The nanoparticles of  $\text{Fe}_x\text{M}_{1-x}\text{S}$  ( $\text{M}=\text{W}, \text{Ni}, \text{Co}, \text{Mo}$ ) and  $\text{FeM}_2\text{S}_4$  ( $\text{M}=\text{Co}, \text{Ni}, \text{Mo}, \text{W}$ ) with different morphologies, nano size, and large active surface area will be decorated on the surface of  $\text{NiCo}_2\text{Se}_4$ . The hetero-structure, multi-atoms and their synergism will facilitate water splitting, the presence of Se in the catalyst will further boost OER which is sluggish in kinetics. These multi-metal chalcogenides will deliver outstanding performance to replace precious metals.

## **Research plan**

The optimize ratio and reaction conditions will be used to synthesize  $\text{NiCo}_2\text{Se}_4$  nanoflowers from the precursor of  $\text{Na}_2\text{SeO}_3$ , Ni and Co Salts. The sample will be tested for morphology, desire composition and activity. In case of unsatisfied results, the precursor will be retreated until to get the best supporting materials. Then the metal salts,  $\text{NH}_4\text{F}$ , and thiourea (in case of  $\text{FeM}_2\text{S}_4$ ) and similarly, acetic acid, sodium hydroxide, metals salts,  $\text{Na}_2\text{S}_2\text{O}_3$  and thiourea (in case of  $\text{Fe}_x\text{M}_{1-x}\text{S}_4$ ) will be simultaneously applied with  $\text{NiCo}_2\text{Se}_4$  nanoflowers, to upload metal chalcogenides on the surface of  $\text{NiCo}_2\text{Se}_4$  nanoflowers. The samples will be tested for morphology, composition, and activity to obtain electrocatalysts with required features. In case the samples are not satisfied we will either go back to initial step of the work or retreat the pre-synthesized  $\text{NiCo}_2\text{Se}_4$  nanoflowers with metal and sulfur precursor to obtain the best electrocatalysts for overall water splitting. After getting the satisfied results the sample will be further studied for application of overall water splitting, investigate HER and OER mechanism and determined the active species for reactions.

## **Broader impact**

Environmental pollution and energy crisis are the hot issues of each community and society around the world. Here, we will develop multi-metal chalcogenides on the surface of metal selenide nanoflower as electrocatalysts for water splitting application. As it will produce hydrogen as energy from very cheap source of water and this may help to resolve energy crisis. In addition, production of hydrogen from water is carbon free process and hydrogen combustion is also a zero carbon emission process. This may help to reduce environmental pollution and provide healthy and safe environment for breath.