

Electrocatalytic water splitting hold great promise for hydrogen production, but their energy efficiency is mainly limited by a slow oxygen evolution reaction (OER) and low accessible active sites in both OER and hydrogen evolution reaction (HER). Most of the electrocatalysts prepared for water splitting are bulk and nanomaterials containing metal oxides, hydroxides, and chalcogenides, etc. However, low atomic utilization at bulk scale, scarcity of noble metals like Pt, IrO<sub>2</sub>, and RuO<sub>2</sub>, can be replaced with the finding of single atom (SA) catalysts. However, the multistep OER at single atomic center and mechanistic pathway for energy intensive -OOH\* pathway requires higher overpotential for OER and in HER too the number of accessible sites are less considering the atomic concentration is usually low under the pyrolytic conditions. The goal of this project is to create high-performance dual atom (DA) bifunctional electrocatalysts with 100% atomic utilization for electrocatalytic water splitting in universal pH conditions. The focus materials are mainly heteronuclear adjacent and O-bridged dual atom catalysts (Pt, Ir, Ru: Ni, Co, Fe,) which will be synthesized through Zeolite Imidazole Framework (ZIF)-8 pyrolysis and electrodeposition (ED). To enhance the exposed active sites, 3D foams such as Nickel foam (NF) will be used to host the dual-atom catalysts via ED, ensuring immobilization and prolonged stability in OER/HER. The prepared cutting-edge dual-atom electrocatalysts will be investigated for electronic and structural properties and will undergo comprehensive characterization. Ultimately, the innovative goal of this project will be compared with existing commercial electrocatalysts in terms of homo- and hetero-nuclear metal DAs, structure-activity relationship for OER/HER for long-term applications. Overall, this proposal addresses critical challenges in clean, compact, and cost-effective energy conversion, fostering knowledge on fundamental aspects of DA catalysts in OER/HER mechanistic pathways. The development of efficient, stable, and affordable electrocatalysts for OER/HER in universal pH conditions will bridge the gap between fundamental and applied electrocatalysis, promoting the advancement of electrocatalytic applications.