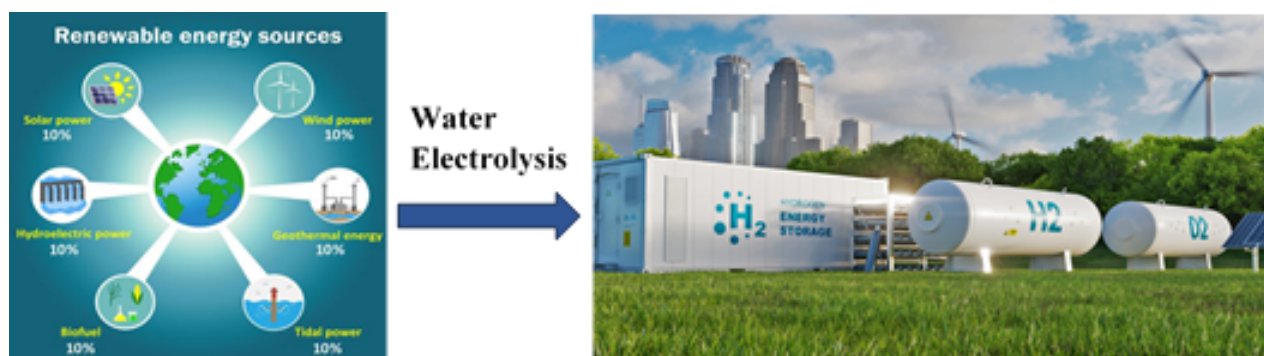


High Entropy Alloy (HEA) Nano Catalysts for Hydrogen Evolution Reaction (HER) through Water-Splitting



KID: 20230412

Global energy demand is rising due to population growth and industrialization, with 85% currently reliant on non-renewable sources. Green hydrogen production addresses energy challenges and offers a zero-carbon fuel alternative.



Hydrogen production through water electrolysis using renewable energy resources

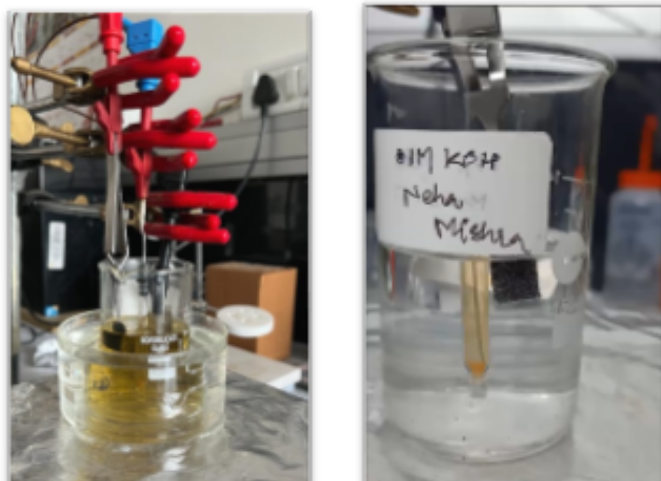
(Source: [renewable-energy-sources-vector-infographics-solar-wind-tidal-hydroelectric-geotherm-in-2023—725501821246507706](https://www.un.org/africarenewal/magazine/july-2022/green-hydrogen-viable-option-transforming-africas-energy-sector).
<https://www.un.org/africarenewal/magazine/july-2022/green-hydrogen-viable-option-transforming-africas-energy-sector>)

Electrocatalytic water splitting is considered a green method of hydrogen gas generation. This process requires a theoretical potential of 1.22V to liberate hydrogen and oxygen at the cathode and anode respectively. Practically, extra potential needs to be applied for the splitting of water which is termed as overpotential. In this context, catalyst plays a crucial role as they have the capability to minimize the overpotential required for the splitting of water. Conventionally, noble metal-based catalysts, especially platinum (Pt) have been used as the most efficient catalyst for the electrolysis of water with fast kinetics in an acidic medium. However, being a noble metal, Pt is very expensive and has limited abundance in nature. On the other hand, commercial catalysts of single metal(s) often suffer from dissolution, aggregation, and sintering resulting in catalyst deactivation. Therefore, there is a need to design inexpensive and novel catalysts that can address the challenges in commercial electrocatalysis for hydrogen evolution reaction (HER) in various alkaline and acidic electrolytes. These electrocatalysts can be designed using computational means such as Density Functional Theory (DFT), Machine Learning (ML), etc. In addition, they can be designed in terms of activity, selectivity, and stability through surface engineering i.e., by changing their sizes (nanosized) and morphologies (nanoparticles, nanowires, and so on). Similarly, structural engineering via alloying, can modify electronic properties by adding other relevant elements. In this direction, nanostructured high entropy alloys (HEA) have come into limelight as promising materials for HER. Based on increased configurational entropy, HEAs are solid solutions consisting of at least five elements in the range between 5 and 35 atomic weights %.

They possess tunable features like composition, electronic structure, and physico-chemical properties like thermal stability, superior corrosion/oxidation resistance, exceptional durability, high hardness, and so on. Very recently, he has been explored in the field of electrocatalysis as a potential candidate for various electrochemical reactions due to their higher activity, stability, and selectivity. Though the combination of various elements provides a huge scope, several challenges starting from fabricating scalable homogeneously distributed composition to alloying of multiple elements are yet to be addressed.

The Combinatorial Lab specializes in the Electrochemical Synthesis of HEA. This is a single-step process involving aqueous-based electrodeposition of multiple elements on some substrate. The lab could successfully synthesize a thin film of FeCoNiCuZn HEA on Ti substrate and the lab's groundbreaking work has resulted in the acquisition of a patent for this unique synthesis route.

The primary goal of our laboratory is to pioneer the development of unexplored (HEA) nanocatalysts specifically designed for the (HER) through water splitting. Our objective is to achieve a remarkable performance in terms of activity, selectivity and stability which will be comparable with commercial Pt/C catalysts (benchmark catalysts). Through this comprehensive approach, our lab aims to make a lasting impact on the field of catalysis, renewable energy, and the transition towards a cleaner and more sustainable energy future.



Electrochemical set-up for HEA synthesis and HER through water-splitting

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Revolutionizing Chemistry for a Sustainable Future: Pioneering Advances in Organometallic Research by OMCL, IITH



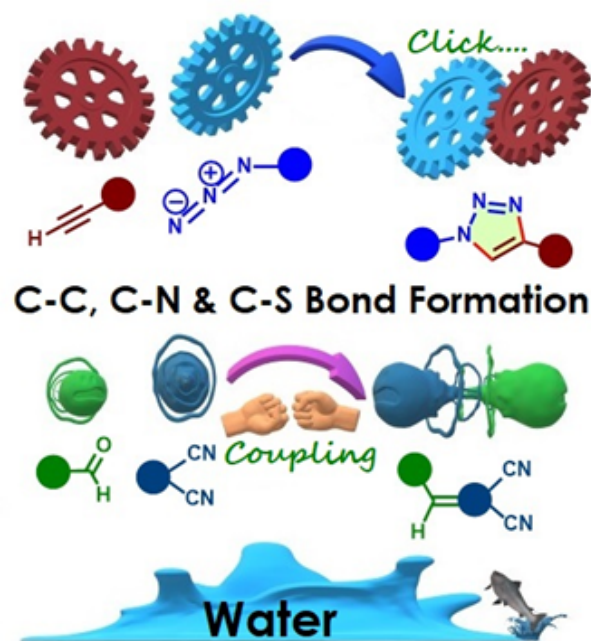
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Our lab is at the forefront of research that unlocks answers to complex questions involving energy, health care, and the environment. We develop significant innovative research and major technological breakthroughs in all aspects of organometallic chemistry and materials, with a particular focus on the important innovation of sustainable methodologies, catalysis, and functional materials.

We contribute to the field of inorganic and organometallic chemistry on fundamental and applied levels by investigating new and efficient ways to activate small molecules and developing catalysts useful in both academic and chemical industries. To accomplish this goal, we systematically develop the hitherto unknown N-heterocyclic carbene (NHC) ligand-supported late transition metal and main group metal catalysts. Novel synthetic methods for metal-NHCs are also being developed within the group, with the aim of making these complexes more attractive for wide-scale use.

We have been Click Chemistry has a great commercial deal in pharmaceutical and life science applications. An azide is added to an alkyne with a copper catalyst. The two reagents click together in a quick and selective manner in the presence of a copper catalyst to result in a single cyclic product. This simple circular economy reaction can be useful in the sustainable synthesis of new drugs through biorthogonal chemistry. This is a key synthetic protocol to generate "clickable" antibodies for cancerous tumours. Based on this technique, antibody-drug conjugates are produced by AstraZeneca and Daiichi Sankyo to replace Herceptin for the treatment of HER2 positive breast cancer.

In this context, we have developed super-fast copper(II) catalyzed click chemistry through a mechanical route to isolate the key pharmaceutical ingredients such as carbazole decorated 1,2,3-triazole derivatives through solvent and additive-free routes. Besides, the regioselective products were isolated within 6 minutes for the first time. This is the only known mild yet fast sustainable approach to isolate the carbazole decorated 1,2,3-triazole derivatives.



GP Group Catalysis Scheme Diagram