Abstract

The transition to sustainable energy systems demands advanced materials for efficient energy conversion and storage to mitigate intertwined environmental pollutions and Energy storage limitations. Emerging strategies focus on zero-emission fuel production such as hydrogen and the design of asymmetric hybrid supercapacitors. Metal–organic frameworks (MOFs), owing to their high specific surface area, tunable porosity, and structural modularity, have emerged a potential candidate. However, intrinsic limitations including low electrical conductivity and chemical instability have prompted researchers to strategically tailored MOFs architecture for enhanced performance. To circumvent these constraints, π-conjugated functional materials are systematically synthesized and incorporated into MOF matrices leading to improved catalytic properties and enhanced electrochemical behavior. This synergistic design significantly advances the performance of MOF-based systems in energy conversion and storage applications. Hence this research centers on strategically synthesis of functionalized conjugated materials as a linkers metal–organic frameworks constructed from various transition metals such as Fe, Co, Ni, Ce and Nd. The successful synthesized materials were characterized by PXRD, BET, SEM (with EDX), DSC/TGA, FTIR and UV-Visible spectroscopy. In project-1 (P-1) and Project-2 (P-2), bimetallic Ni/Co and Ni/Fe MOFs architecture were synthesized using 2,5-dihydroxyterephthalic acid (DHTA) as linker and MOFs architecture exhibited excellent catalytic activity for water splitting, underscoring their potential as efficient electrocatalysts for energy conversion applications. In project-3 (P-3), Ce/Co-based MOFs were synthesized using 5,10,15,20-Tetrakis (4-carboxy phenyl) porphyrin (TCPP) as a linker to investigate their potential application in OER and energy storage applications especially in asymmetric hybrid supercapacitors. The resulting MOFs architecture demonstrated excellent catalytic activity in supercapacitor devices as well as in OER. In Project-4 (P-4), Ce/Nd-based MOFs were synthesized using 4,4'-(Benzo[c]thiadiazole-4,7- diyl)dibenzoic acid as a linker to investigate their behavior in energy storage applications. The resulting MOFs architecture demonstrated promising electrochemical performance, highlighting their suitability and versatility for advanced energy storage systems. In Project-5 (P-5), Ni/Co- based MOFs were synthesized using 5-(5-carboxy-*1H*-pyrrol-2-yl)picolinic acid and 5-(4- carboxyphenyl)-*1H*-pyrrole-2-carboxylic acid as ligands for their potential applications in water

splitting. Both the bimetallic metal-organic frameworks exhibited promising catalytic activity for hydrogen and oxygen generation in HER and OER respectively.

This study underscores the critical role of ligand engineering and metal selection in optimizing MOF-based materials to offer a promising pathway for the development of efficient energy conversion and storage technologies.