

ABSTRACT

The growing global energy crisis and environmental concerns highlight the urgent need for green and sustainable energy to substitute fossil fuels. Hydrogen (H_2), with its exceptionally high energy density and zero-carbon emissions, stands out as a promising clean fuel. MOFs are highly porous materials with large surface areas, tunable pore structure and high crystallinity ideal for potential applications. This research includes designing and synthesizing of organic ligands (4,4'-(benzo[c][1,2,5]thiadiazole-4,7-diyl)dibenzoic acid) and 4,4'-(quinoxaline-5,8-diyl)dibenzoic acid) by Suzuki coupling reaction in the presence of Tetrakis(triphenylphosphine) palladium as a catalyst. Organic ligand combines with Zinc salt under solvothermal condition to yield MOFs (Zn-BTDB) and (Zn-QxDB). The prepared ligands and their MOFs were characterized by UV-Vis spectrophotometry and Fourier Transform Infrared spectroscopy. Computational studies provide insights into their electronic properties, reactivity parameters and electron-hole distributions highlighting the role of organic ligands in metal-organic frameworks. Electrochemical evaluation reveals that Tafel Slope of MOF (Zn-BTDB) is 49.01mV/dec at a current density of 10mA/ cm^{-2} with an overpotential of 315mV for OER (oxygen evolution reaction) while 205.9mV/dec Tafel slope with an overpotential of 16.4mV for HER (hydrogen evolution reaction) indicating excellent catalytic activity. The results proved that Zn-BTDB MOFs are good for water splitting application.