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Comparison of the catalytic activity of a zirconium-based metal-organic framework and its defective structure in hydrogen production

In this research, a zirconium-based metal-organic framework (MOF-801) and its post-synthetically produced modified structure (Quasi-801) were used to access unsaturated metal centers as active catalytic sites for hydrogen gas production using sodium borohydride (NaBH4). For this purpose, the zirconium-based metal-organic framework was first synthesized in dimethylformamide (DMF) solvent. Then, through controlled thermal treatment, the structure was modified, and the related quasi- metal-organic framework with unsaturated metal sites was created. The presence of these metal sites as Lewis acids in the catalytic reaction of hydrogen production from the hydrolysis of sodium borohydride proved to be effective and increased the catalytic efficiency. Additionally, the effects of temperature change on the catalytic activity of the metal-organic framework (and its modified structure) and the amount of hydrogen produced were investigated. An increase in reaction temperature activates some of the metal sites that are inactive at lower temperatures. Consequently, thermal modification added to the number of available sites for hydrogen production, two-fold increasing the process yield. According to the results, the thermal modification process effectively impacts the catalytic performance of the structure and improves the catalytic behavior of the structure. Therefore, the development of quasi- metal-organic frameworks can be an attractive method for developing hydrogen production catalysts as a clean fuel.

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