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Biphenyl monolayer construction with single transition metal doping as electrocatalysts for conversion CO_2 to fuel

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ABSTRACT

Developing sophisticated electrocatalysts is crucial in capturing chemically unreactive CO_2 and transforming it into valuable products like fuel. This is essential for effectively tackling the issues of energy crisis and greenhouse gas emissions while maintaining considerable sustainability standards. Nevertheless, effectively managing the selectivity of products while maintaining a small overpotential remains a challenging task. Present work utilized density functional theory (DFT) for studying electrocatalytic potential of various single transition metals (TMs), such as cobalt, iron, and manganese, in process of carbon dioxide reduction reaction (CO_2RR). Effectiveness of CO_2RR was evaluated for each TM by analyzing their interaction with reaction intermediates (CHO, CO, and COOH) when incorporated into biphenyl monolayer (BPM) systems. Based on the analysis of ΔE values and barriers, it was determined that incorporating Fe into the biphenyl monolayer system is the most efficacious approach for the CO_2RR to generate methane. This configuration achieves an exceptionally low overpotential potential (U_L) of −0.36 V. In hydrogen evolution reaction (HER), it was observed that CO_2 exhibits a higher affinity for occupying the activation site on Fe-BPM compared to H_2. This difference in adsorption energy (E_{ad}) (−0.94 eV for CO_2 vs. −0.43 eV for H_2) highlights their distinct behaviors. Additionally, Fe-BPM effectively suppresses the HER during the CO_2RR process, as indicated by the HER's U_L of −0.43 V. Findings of present study are anticipated to provide a novel direction in the advancement of electrocatalysts with low potential, while simultaneously exhibiting remarkable selectivity and activity for CO_2RR.

1. Introduction

Different energy storage materials are being explored currently for their portable and automotive applications [1–4]. The electrochemical process of carbon dioxide reduction reaction (CO_2RR) holds significant promise for conversion and employing carbon dioxide. By utilizing

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