THEORETICAL STUDY OF THE CATALYTIC PERFORMANCE OF Fe AND Cu SINGLE-ATOM CATALYSTS SUPPORTED ON Mo_2C TOWARDS THE REVERSE WATER-GAS SHIFT REACTION (RWGS)

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The reverse water gas shift (RWGS) is an attractive process using CO_2 as a chemical feedstock. Single-atom catalysts (SACs) exhibit high catalytic activity in several reactions, maximizing the metal use and enabling easier tuning by rational design than heterogeneous catalysts based on metal nanoparticles. In this study, we evaluate, using DFT calculations, the RWGS mechanism catalyzed by single-atom catalysts (SACs) based on Cu and Fe supported on Mo_2C, which is also an active RWGS catalyst on its own. While Cu/Mo_2C showed more feasible energy barriers toward CO formation, Fe/Mo_2C presented lower energy barriers for H_2O formation. Overall, the study showcases the difference in reactivity between both metals, evaluating the impact of oxygen coverage and suggesting Fe/Mo_2C as a potentially active RWGS catalyst based on theoretical calculations.