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A Density Functional Theory Study of Formic Acid Formation from CO2 Hydrogenation over Au-exchanged MCM-22 Zeolite

One of the important goals in energy and environmental research is to find novel materials to sequestrate and convert greenhouse gases to useful chemicals. In this study, the well calibrated Density Functional Theory (DFT) is used to study the adsorption of CO2 and H2 in order to investigate possible reaction pathways for CO2 hydrogenation to formic acid over gold supported MCM-22 zeolite catalyst. The adsorption energies of CO2 and H2 on Au-MCM-22 catalyst are −15.2 and −30.4 kcal/mol, respectively. From the order of adsorption, two possible reaction mechanisms are proposed. The first mechanism, hydrogen molecule is first adsorbed on gold and zeolite, resulting in gold hydride and Brønsted acid site of zeolite. Formic acid is consecutively formed via the protonation of CO2 over the Brønsted acid and simultaneous formation of the bond between CO2 and the hydride group. The activation energy of the rate determining step of this pathway is 39.5 kcal/mol. In the second mechanism, CO2 is primarily interacted over the active site. The hydrogen is co-adsorbed and reacted with CO2 to produce intermediate adsorbing on Au. The activation energy of this step is 40.5 kcal/mol. The hydrogen transfer to HCOO intermediate to generate formic acid is proposed in the last step. Due to these comparable pathways at least at high temperature, both the reaction mechanisms could therefore be possible, depending on the order of adsorption. Accordingly, the gold-exchanged MCM-22 zeolite could be potentially used as the catalyst for producing formic acid from CO2 and hydrogen molecules.

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