A theoretical study of carbon dioxide hydrogenation to methanol on Ni$_2$P (001) surface

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Abstract: Carbon dioxide (CO$_2$) is one of main greenhouse gases (GHG) released from fossil fuels. The conversion of CO$_2$ to valuable chemicals such as formic acid, formaldehyde and methanol has received much attention from industrial sector. In this work, the reaction mechanism of CO$_2$ hydrogenation to valuable chemicals on Ni$_2$P (001) surface has been investigated by means of the density functional theory (DFT). The possible reaction pathways are considered to proceed via either the formate (HCOO) or hydrocarboxyl (COOH) pathways. For the formate pathway on Ni$_2$P surface is suggested as CO$_2$ → H$_2$* + CO$_2$ → H* + HCOO* → HCOOH*, followed by the hydrogenation to form formaldehyde and methanol as the products. The hydrocarboxyl pathway is involved with the COOH*, COOH* and CH$_2$OH* as intermediates and the hydrogenation to form methanol as the product. The calculation results provide the basis for exploring the nature of Ni$_2$P catalysts in the hydrogenation of CO$_2$ involved in the greenhouse gas reduction, and the conversion of greenhouse gases.

Keywords: Carbon dioxide; Ni$_2$P; Hydrogenation; Density functional theory