

A first principles study of carbon monoxide hydrogenation on cobalt (001) surface.

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Carbon monoxide (CO) is a colorless, odorless, and non-irritable gas [1]. Fischer–Tropsch synthesis (FTS) is a process that has been used for many decades as it gives access to industrially important chemicals from CO [2]. As the products of FTS are a complex mixture of a wide range of organic compounds, selectivity toward desired products is the most important issue in this reaction. In recent years, there has been an increasing motivation to deploy FTS at commercial scales, which has fueled the search for high-performance catalysts [3]. Several catalysts have been examined for their potential to catalyze CO hydrogenation. Transition metal catalysis has long been recognized as a reliable and modular means of constructing complex molecules from simple, readily accessible starting materials[4]. Periodic plane-wave density functional theory (DFT) calculations were carried out to study the CO adsorption and its reactivity with adsorbed hydrogen on the Co (001) surface. All parts of this study employed the Vienna Ab initio Simulation Package (VASP) [5]. The results show that CH₄, CH₃OH, and C₂H₂ are the products, according to the calculations CH₄ is the main product. We found that the preferred mechanism for CO hydrogenation is through HCO and cis-HCOH, and the largest exothermic reaction energy in the CH₄ formation pathway is released during the hydrogenation of cis-HCOH (−0.773 eV). An investigation of the kinetics demonstrates that the CH production from cis-HCOH has the lowest energy barrier. On the other hand, the hydrogenation of CO to COH is the least favored reaction kinetically.

Keywords: Carbon monoxide; Fischer–Tropsch Synthesis; Cobalt catalyst; DFT

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