22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

DFT study on the hydrogenation of carbon monoxide on a SiO_2-based catalytic surface

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The increasing demand to obtain clean fuels and useful products has created an interest in finding active and selective catalysts for the conversion of carbon monoxide into desired products. The hydrogenation process of carbon monoxide is often polymerized into liquid hydrocarbon chains using catalysts. In this research, density functional theory (DFT) [1] calculations have been used to investigate the reaction mechanism of Fischer-Tropsch synthesis on silica-based catalytic surfaces. [2] Silicon dioxide is known as a catalytic substance that can be a suitable surface for hydrogenating the carbon monoxide molecule and thus reducing the amount of pollutants in the atmosphere. 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) [3]. After examining the paths of methanol and methane production, it was found that the exothermic methanol production and the COH production stage in it are the rate-determining steps, and in the case of the methane path, which is an endothermic process, the CH + H step is the rate-determining step. The results show that methane formation is more favorable compared to other products.

Keywords: Carbon monoxide, Fischer–Tropsch Synthesis, DFT, SiO_2

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