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THE THERMODYNAMICALLY INVESTIGATION OF ETHYLENE/ETHANE FORMING PROCESS FROM ETHYL ON IRON(100) SURFACE USING DFT

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Abstract: Today, energy crisis is one of the most important human problems, while oil reserve of many countries, including Iran is dwindling. But, the advent and advancement of technology through the conversion of Gas-Synthesis (a mixture of CO and H) into liquid hydrocarbons, by Fischer-Tropsch synthesis (FTS) is more promising future in this field. Metals such as cobalt, nickel, zinc and iron are used as catalysts for FTS. Studies have shown that the metal catalyst surface structure has a great influence on the process, and leading to different products and transition states. Iron is known the most used and the most cost-effective metal catalyst in FTS. Different surfaces of Iron have different catalytic roles. In our work, Fe(100) -that is the most stable after Fe(110) and is known as the most active iron's surface in FTS- was selected and a theoretical investigation of adsorption energy for formation of ethylene and ethane from a reaction between ethyl radical and H, using Density Functional Theory (DFT). The resulted data suggests that the ethylene adsorption versus alkane adsorption is thermodynamically preferred on Fe(100).

Keywords: Fischer- Tropsch Synthesis, DFT, Fe(100), Ethylene, Ethane.

1. INTRODUCTION

Fischer and Tropsch reported for the first time in 1923 the synthesis of liquid hydrocarbons by means of the CO hydrogenation on an alkalised-iron catalyst [1]. Furthermore, the investigation of fundamental adsorption and reaction properties of hydrocarbons on metal single crystal surfaces under ultra-high-vacuum conditions has become part of the foundation as well as a significant avenue towards the progress of modern surface science and catalysis.

There are typically three popular FTS mechanisms [2], although much debate on the subject still lingers on. The most accepted is the *carbide mechanism* which entails CO adsorption and dissociation towards adsorbed carbon and oxygen atoms, as well as successive hydrogenation of surface carbon atoms towards CHx fragments, and insertion of CHx monomers into the metal-carbon bond of an adsorbed alkyl chain. With methyl as chain initiator, methylene is considered the frame-building