

Computational Investigation of Fischer-Tropsch Synthesis on Alkali-Promoted Iron Carbide Catalysts

Background

Fischer–Tropsch synthesis (FTS) is a heterogeneous catalytic reaction, in which synthesis gas (a mixture of carbon monoxide (CO) and hydrogen (H₂)), is converted into desired fuels and chemicals. Fe is one of the main components of the active phase of industrial FTS catalysts due to its low price and high activity. The evolution of the active phase of Fe-based catalysts is very complex, resulting in considerable debate on the nature of the active phase and on the FTS reaction mechanism for Fe-based catalysts.

Recently, it was reported that pure iron carbides showed attractive catalytic performance in selectivity and activity. Wang et al. achieved the synthesis of phase-pure ϵ (')-Fe_{2(2.2)}C and showed that high stability and a near-zero CO₂ selectivity under industrial FTS conditions. Due to the excellent catalytic performance of the ϵ (')-Fe₂C phase, it is worthwhile to investigate the mechanism of the conversion of syngas to products such as olefins and paraffins. There are few researches focused on the influence of promoters on these Fe carbides. Typically, alkali metals are used as promoters, because they can enhance the catalytic performance in terms of activity and product distribution. Moreover, some studies indicated that the use of alkali metals as a promoter into Fe-based catalysts for FTS can enhance catalyst stability and promote the WGS reaction. Despite these experimental indications, there are only limited theoretical studies into the enhanced activity of iron carbides promoted by alkali metals catalysts for FTS.

The goal of this project is to investigate the influence of alkali promoter on the relevant elementary reaction steps in CO hydrogenation on the most important Fe-carbide. Potential energy surfaces will be constructed for such models, the associated electronic structures will be analyzed and the impact on CO hydrogenation will be assessed by microkinetic modeling.



Research objectives:

- DFT calculations of relevant reaction pathways of CO hydrogenation on Fe-carbides with a specific focus on the impact of alkali metals.
- Investigation of the reverse water-gas shift (RWGS) reaction .
- Microkinetic analysis of CO hydrogenation and WGS/RWGS reactions.

For further information:

Emiel Hensen (Helix, STW 3.33), Tel 5178, e.j.m.hensen@tue.nl

Ivo Filot (Helix, STW 3.39), Tel 4952, i.a.w.filot@tue.nl

Xianxuan Ren (Helix, STW 3.38), x.ren4@tue.nl

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