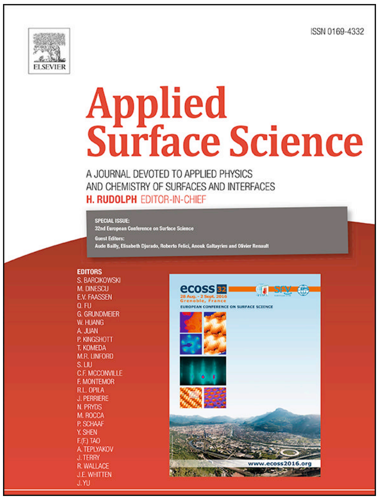

Full Length Article

Insight into the Role of the Promoters Pt, Ru and B in Inhibiting the Deactivation of Co Catalysts in Fischer-Tropsch Synthesis

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Insight into the Role of the Promoters Pt, Ru and B in Inhibiting the Deactivation of Co Catalysts in Fischer-Tropsch Synthesis

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Abstract: In order to probe into the roles of the promoters Pt, Ru and B in inhibiting the deactivation of Co catalysts in FTS reactions, the adsorption ability of neighboring surface C and subsurface C atom around the promoters (Pt, Ru and B), and the mechanisms of surface C diffusion, accumulation, hydrogenation and penetration are examined by density functional theory calculations over the promoters Pt, Ru and B-modified Co catalysts, as well as the pure Co catalysts. Our results clearly show that compared to Co catalysts, both PtCo and RuCo bimetallic catalysts promote surface C hydrogenation, and inhibit surface C diffusion, accumulation and penetration, and therefore the ability of resistance toward deactivation and the stability of Co-based catalysts are enhanced; the promoter B cannot effectively improve the ability of resistance toward deactivation. Thus, the sequence for resistance toward deactivation of Co-based catalyst is BCo<Co<PtCo<RuCo. Moreover, the activation free energy of surface C accumulation to C_2 species increases with the increasing of surface C adsorption free energy, namely, the adsorption characteristic of surface C species well represent the surface carbon deposition. Our results not only give an explanation for reported experiment that the Pt, Ru and B-modified Co catalysts exhibit ability of resistance toward deactivation in FTS at a molecular level, but also provide a clue for the design of efficient Co-based catalysts in FTS reactions.

Keywords: Cobalt, Fischer-Tropsch synthesis, Promoter, Deactivation, Density functional theory

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