The effect of Co-promotion on MoS2 catalysts for hydrodesulfurization of thiophene: A density functional study - DTU Orbit (10/12/2018)

The effect of Co-promotion on MoS2 catalysts for hydrodesulfurization of thiophene: A density functional study

We present density functional theory (DFT) calculations of the hydrogenation (HYD) and direct desulfurization (DDS) pathways of thiophene hydrodesulfurization (HDS) over cobalt-promoted MoS2. We find that the Co–Mo–S edge in its equilibrium state under HDS conditions is reactive toward both hydrogenation and C–S bond scission without the initial creation of vacancies. This can be accomplished such that additional S is bound to the Co–Mo–S subsequent to C–S bond scission and then removed in the final reaction step. We find thus that coordinatively unsaturated sites (CUS) are present in the equilibrium structure, and at these sites HDS can take place without sulfur removal in the first step. No traditional vacancies are formed and the present mechanism is therefore very different from the previously proposed vacancy mechanisms requiring the initial creation of a sulfur vacancy for the reaction to proceed. We find that Co-promotion decreases the barrier of hydrogenation reactions and active site regeneration but increases the barrier of C–S-scission reactions. The net result of Co promotion is found to be an increase in the hydrogenation activity and also of the relative importance of the DDS pathway. We compare our results to available experimental information and find a number of consistencies and parallels. Therefore, we can rationalize the promoting effect of Co such that at the Co–Mo–S edge, good hydrogenation properties are combined with the ability to bind additional sulfur upon C–S-scission. Finally, we propose that the interactions between the Co-promoted S-edge and the non-promoted Mo-edge may play a role in the hydrogenation pathway.

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