A theoretical explanation of the effect of oxygen poisoning on industrial Haber-Bosch catalysts - DTU Orbit (25/04/2019)

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The Haber-Bosch process has been studied extensively, yet a low-temperature, low-pressure process remains elusive. As has been shown many times, this stems in part from the difficulty of breaking the N-N triple bond. In this work, we highlight an additional reason for the lack of a low-temperature ammonia synthesis process: the effect of oxygen poisoning at low temperature. Using density functional theory (DFT), we have created a new model for the active site of industrial Haber-Bosch catalysts which explicitly includes the potassium promoter. Furthermore, we present a new micro-kinetic model for ammonia synthesis that includes the effect of oxygen poisoning due to trace water content in the input gas stream. Our model agrees well with previous experiments and shows that devising a strategy to avoid oxygen poisoning is crucial to creating a low-temperature Haber-Bosch process. Additionally, the model suggests that using a weaker-binding catalyst is one way to avoid oxygen poisoning if it is impractical to remove all water from the reactor.

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