Inorganic Materials & catalysis

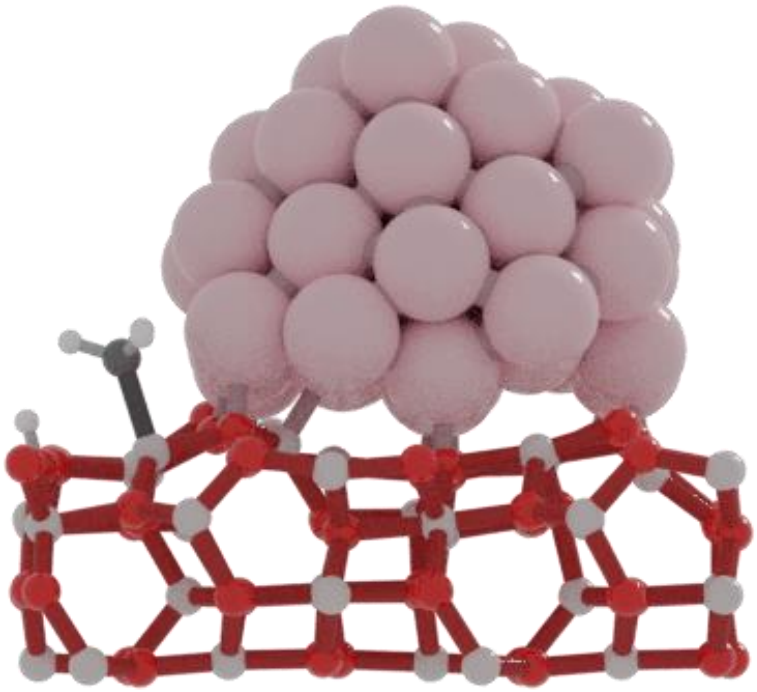
Research Project – Emiel Hensen/Ivo Filot/Roos Krösschell

INORGANIC MATERIALS & CATALYSIS

Support effects in methanation on cobalt

Background

Catalysts on different supports show different behaviour. To elucidate the undesired formation of methane in Fischer-Tropsch synthesis at the metal-support interface and what role the support plays in the methane formation, reaction pathways from CO to methane on cobalt clusters on various supports are investigated. Direct and hydrogen-assisted routes are investigated. The supports include titania and ceria (reducible oxides) and alumina and silica (non-reducible oxides). The pathways on these supported cobalt nanorod will be investigated. This nanorod includes a B_5 site. The pathways on these systems can be compared to the pathways on cobalt nanorods supported by other metal oxides.



Techniques used:

Computational techniques will be used to obtain the data needed for this project. First principles electronic structure calculations using DFT will be done to calculate the stability of configurations and to calculate energy barriers. COHP (crystal orbital Hamilton population) and DOS (density of states) analyses will be performed to rationalize the results obtained with DFT. Microkinetic modelling will be used to light up the most important steps in the mechanism. The connection with experiments will be made. This way, the obtained computational results will play a key role in interpreting several experimental results.

Learning goals:

- Deepen chemical understanding of reaction mechanisms and interactions between atoms and molecules.
- Enhance creative thinking in formulating and investigating possibilities that could account for observed (experimental) outcomes.
- Perform different kinds of DFT calculations in VASP.
- Use scientific method to formulate research questions, design experiments and process and interpret the output data.

For further information:

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