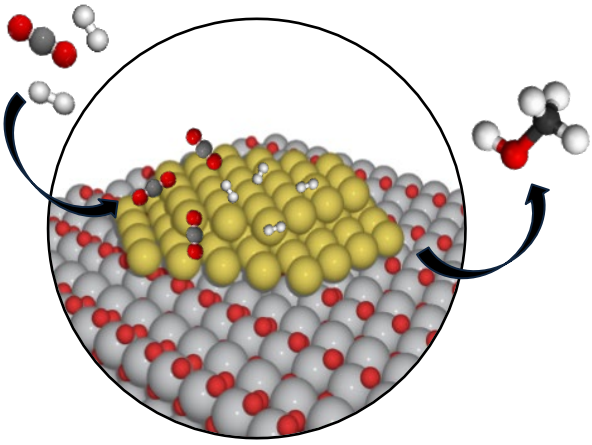
Inorganic Materials & Catalysis
Molecular Heterogeneous Catalysis
Research Project:
Ivo Filot/Emiel Hensen/Francesco Cannizzaro

INORGANIC MATERIALS & CATALYSIS

CO_2 hydrogenation to methanol on In_2O_3 catalysts



Catalytic conversion of CO_2 and hydrogen to methanol represents a central technology for CO_2 utilization and an economically viable way to alleviate global warming. However, such transformation is challenged by the difficulties associated with the chemical activation of CO_2. The current generation of industrially applied heterogeneous catalysts mainly relies on Cu-based systems, which usually show low catalytic activities, are selective for the undesired reverse water-gas shift reaction and are easily deactivated by the H_2O by-product. Recently, defective-oxides materials, such as In_2O_3, have emerged as promising catalysts for methanol synthesis from CO_2 as they show higher selectivity to methanol. It is suggested that the presence of oxygen vacancies on the catalyst's surface enhances CO_2 adsorption and activation. Despite initial promising results, current formulations still suffer from low activities and cannot be scaled up to the level of industrial processes. By means of theoretical simulations, it is possible to investigate how to tune the catalyst formulation in order to optimize catalytic performances ultimately aiming at better chemical processes.

In this project, we aim at investigating the mechanism of adsorption and surface reaction for CO_2 hydrogenation to methanol on an $In_2O_3(111)$ surface. By incorporation of various transition metals (e.g. Ni, Pd, and Co) and oxides (ZrO_2) into the In_2O_3 lattice, we will also investigate the promotional effect of those materials on the formation of oxygen vacancies as they are considered to be the active sites for the CO_2 activation. Furthermore, we also wish to investigate the activity for CO_2 hydrogenation to methanol at the interface between transition metal nanoparticles and In_2O_3

Project-specific learning goals:

- Perform DFT calculations to explore stable structures and elementary reaction steps.
- Develop microkinetic modelling simulations to investigate the reaction mechanisms.

Tasks:

During the project you will be made familiar with scientific computing techniques. These will include (a) geometry optimization of structures; (b) searching reaction pathway and understand the catalytic activity; (c) thermodynamic analysis and microkinetic simulation; (d) electronic and vibrational analysis including Density of States (DOS), and Bader charge analysis.

General learning goals:

- Formulate relevant research questions.
- Construct a working hypothesis.
- Develop a scientific methodology to validate or invalidate the working hypothesis.
- Write a research report based on the research carried on.
- Present the most salient results in an oral contribution.

For further information:

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