Inorganic Materials & Catalysis
Molecular Heterogeneous Catalysis
Research Project:
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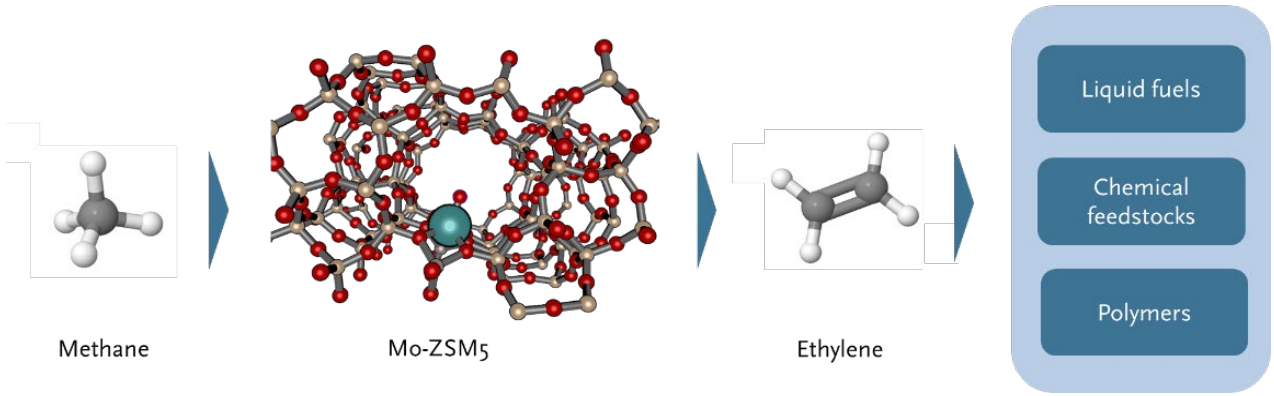
Direct methane-to-hydrocarbons conversion on HZSM-5 zeolites

For its low carbon emission per energy unit of methane, natural gas is nowadays considered as a promising transitional energy source to help the transformation of the current industrial and energy systems towards more sustainable ones. Furthermore, methane can act as feedstock to synthesize crucial building blocks for the chemical industries. In this context, technologies able to convert methane into liquid hydrocarbons are highly desirable, as these would (1) enable easier transportation of this resource making it more accessible to the chemical industry and (2) help the transition towards a more sustainable industrial production.

In this project, we aim at investigating the chemo-kinetic network for CH_4 conversion to highly-valuable products such as ethylene and methanol over ion exchanged zeolites. By introduction of transition metals (e.g. Co, Ni, Cu, Fe) into the zeolite cages, we will investigate the nature of the active phase and the influence of the metals on activity and selectivity.



Project-specific learning goals:

- Perform DFT calculations to explore stable structures and elementary reaction steps.
- Develop microkinetic modelling simulations to investigate the reaction mechanisms.
- Connect theoretical simulations to carefully conducted kinetic measurements in the laboratory.

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 also 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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