Inorganic Materials and Catalysis

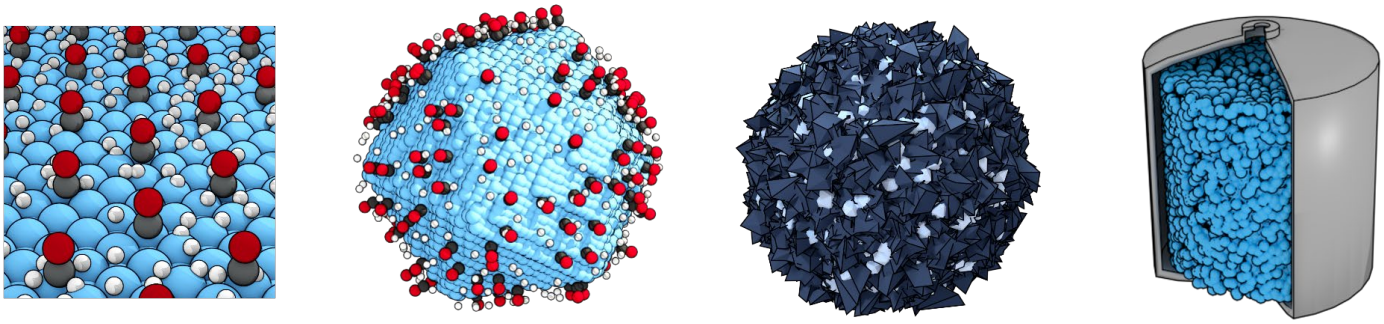
Research Project – Emiel Hensen/Bart Klumpers/Ivo Filot

IMC
INORGANIC MATERIALS & CATALYSIS

Understanding multiscale catalysis with artificial intelligence

Background

A major challenge in understanding catalytic processes stems from their intrinsic multiscale nature. The chemical activity of a catalyst is principally attributed to a selection of atomically defined sites. These sites are distributed over different nanoparticle facets, which in turn are embedded in mesoporous support pellets inside chemical reactors. Modelling of these systems requires accurate descriptions of processes occurring at every level. This promotes the use of multi-model approaches, each tackling one particular domain. The challenge is then to determine the multiscale phenomena relevant to each domain in order to bind the different models together.



Direct integration of the different models (such as electronic structure calculations, microkinetics or reactor simulations) is restricted by computational limitations. This has resulted in the development of many approximate models, seen with force-fields or lumped kinetics, which provide a trade-off in their accuracy to improve computational cost. However, these models tend to only be viable in a small application regime, which makes it difficult to reliably describe multiscale phenomena.

In recent years, machine learning has provided new opportunities to replace these traditional models. Machine learning models provide better flexibility in capturing the features of our catalytic systems, while also avoiding bias due to modelling assumptions. They can be applied to describe the catalyst across the full operating regime, with negligible loss of accuracy (and low cost to boot). The challenge then, lies in the model construction itself:

- How do we efficiently teach chemical and catalytic principles to a machine?
- How to deal with the large amounts of data (terabytes!) generated by our models?

Overcoming these challenges, we can observe processes taking place at much larger scales than before:

- Directly observe reaction and diffusion processes across catalytic surfaces
- Analyse changes in activity and selectivity through the cross-section of the catalyst particle
- Observe how temperature gradients in the reactor influence the microkinetics

Potential projects

- Analysis of surface reactions for the construction of microkinetic models
- Prediction of site distributions and/or catalyst nanoparticle shapes
- Integration of microkinetics in reactor or particle models

For further information

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