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Coach	**Supervisor(s)**	**Funding**
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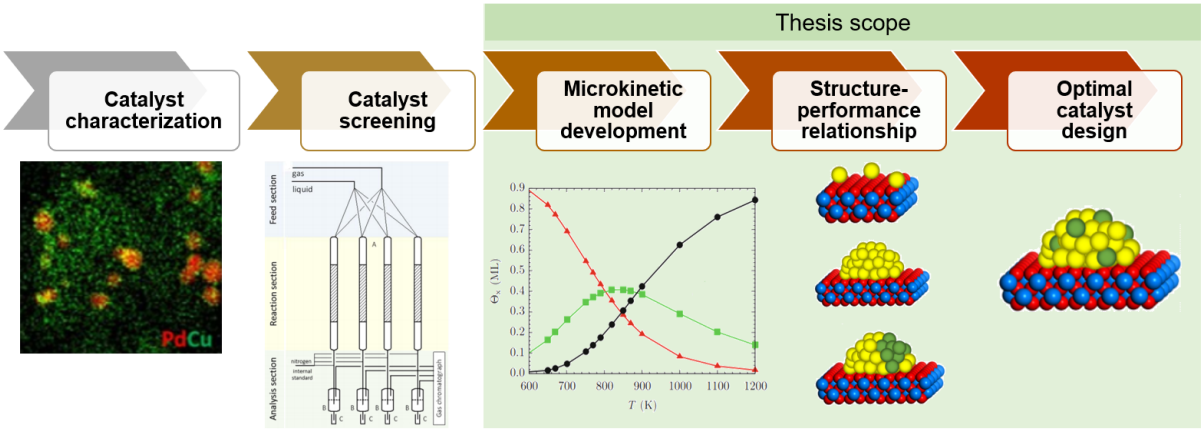
Model-driven catalyst design for ethanol dehydration into ethylene

Aim

Construction a kinetic model for ethanol dehydration, which includes all measurable physico-chemical properties of experimentally tested catalysts and allows for the establishment of catalyst structure-activity relationships. Testing of virtual catalysts and propose an optimal catalyst composition for maximizing the ethylene yield.

Justification

Ethylene is one of the largest chemical products in the world and a very important building block. Next to polyethylene, numerous petrochemical products are obtained from ethylene such as acetic acid, styrene, acetaldehyde, ethylene glycol, ethylene oxide, vinyl chloride etc. About 99% of ethylene is produced from cracking of hydrocarbons. However, fossil-based production faces numerous problems with respect to the environment and depletion of crude resources. Ethanol dehydration is seen as a promising greener alternative for ethylene production. It has been intensively studied in recent years in terms of catalyst screening and mechanism elucidation. Experimental data on ethanol dehydration has been collected previously for a variety of ZSM-5 catalysts at temperatures ranging from 440 to 620 K.[1] Model-driven design of heterogeneous catalysts is a new and promising methodology to optimize catalytic material performances.[2] Therefore, a microkinetic model, including all measurable catalyst characteristics (e.g. number of active sites, distribution of active sites, acid strength), has to be developed based on the previously acquired experimental data. Regression against experimental data, then, provides values for the kinetic and catalytic descriptors, describing the link between the catalyst characteristics and resulting performance. Once the relationships are established, a set of virtual (i.e. testing beyond experimentation) catalysts will be formulated in other to find the optimal set of descriptors, and catalyst properties, to optimize the process, i.e., maximize the ethylene yield.



Program

- Identification of the relevant catalyst characteristics to be included in the microkinetic model.
- Construction of the microkinetic model for ethanol dehydration and regression to the experimental data to determine the catalyst descriptors, enabling structure-activity relationships.
- Formulation of virtual catalysts and screening of the ethanol dehydration performance.
- Propose an optimal catalyst design to maximize ethylene yield during ethanol dehydration.

References

1. Van der Borght K, Toch K, Galvita VV, Thybaut JW, Marin GB. Information-driven catalyst design based on high-throughput intrinsic kinetics. *Catalysts.* 2015;5(4):1948-1968.
2. Pirro L, Mendes PSF, Paret S, Vandegehuchte BD, Marin GB, Thybaut JW. Descriptor–property relationships in heterogeneous catalysis: exploiting synergies between statistics and fundamental kinetic modelling. *Catalysis Science & Technology.* 2019;9(12):3109-3125.

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