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Active Learning for Prediction of Adsorption Enthalpies in Zeolites

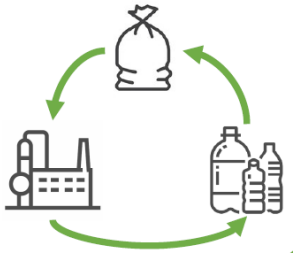
Keywords

Aim

Develop a machine learning model for prediction of adsorption enthalpies in various zeolite frameworks to facilitate model-guided catalyst design for the catalytic conversion of plastic waste to olefins.

Justification

With an annual production of 350 Mt plastics, the recycling of plastic waste will be one of the crucial challenges for the chemical industry to achieve climate neutrality [1]. *Ex-situ* catalytic pyrolysis of polyolefins is a promising technology for the conversion of waste polyolefins to high-valuable light olefins. Subsequently, these olefins can be converted into virgin polymer or other valuable base chemicals, which closes the loop for polyolefin waste.



The development of improved catalysts that enhance both the activity and selectivity towards olefins is one of the main areas of interest for the industrialization of catalytic pyrolysis. Therefore, first-principle kinetic models are developed to determine the effect of the zeolite structure on the reaction yields. The adsorption enthalpy and entropy of the adsorbed hydrocarbons are one of the main determining properties of how the zeolite influences the product yields. Therefore, a good understanding of these adsorption properties is essential for model-guided catalyst design. At present adsorption enthalpies are only determined for a limited number of linear alkanes or alkenes in a selective range of zeolites [2]. Moreover, current models are based on linear regression and have a limited range of application.

Machine learning techniques allow to model the complex relation between adsorbent, zeolite and the adsorption enthalpy but require an extensive amount of data. Active learning allows to reduce the number of data required by letting the machine learning algorithm decide which data is the most interesting to acquire. DFT-calculations in VASP will be used to determine the adsorption properties of the hydrocarbons and so further facilitate model-guided zeolite design.

Program

- Literature study on current methods for the prediction of adsorption enthalpies and zeolite representation in machine learning
- Development of molecular and zeolite representation to allow property prediction
- Determine DFT-based adsorption enthalpies for representations selected by active learning
- Training and evaluation of machine learning model for adsorption property prediction

References

[1] Lange JP. Towards circular carbo-chemicals – the metamorphosis of petrochemicals. Energy & Environmental Science 2021;14(8):4358-76.

[2] De Moor BA, Reyniers M-Fo, Gobin OC, Lercher JA, Marin GB. Adsorption of C2− C8 n-Alkanes in Zeolites. The Journal of Physical Chemistry C 2011;115(4):1204-19.

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