From Ångstroms to meters: on the Role of Multiscale Modelling in Heterogeneous Catalysis

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The successful development and application of heterogeneous catalysts requires knowledge and expertise on multiple length scales ranging from the atomistic and molecular scales, on which the breaking of chemical bonds and the interaction between individual molecules are considered, to the particle and reactor scale, on which mass and heat transport influence the catalytic conversion of molecules. Although sophisticated numerical models have been developed on both ends of the spectrum, e.g., Density Functional Theory (DFT) models on the atomistic scale and Computational Fluid Dynamic (CFD) models on the reactor scale, the combination of different models into a multiscale model is still challenging. Multiscale models in particular allow to explore different phenomena on different length and time scales and thus to understand the links between the different scales in heterogeneous catalysis. Consequently, they are a promising tool to gain further insights into the full catalytic cycle.

In this talk, a brief introduction to multiscale modeling in heterogeneous catalysis is presented. Afterwards, examples that highlight the value of modeling in heterogeneous catalysis are discussed, and an outlook on the chances and challenges of multiscale modelling for biobased catalysis is given.