Knowledge-Based Approaches in Catalysis and Energy Modelling

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Reflecting the general data revolution, knowledge-based methods are now also entering theoretical catalysis and energy related research with full might. Automatized workflows and the training of machine learning approaches with first-principles data generate predictive-quality insight into elementary processes and process energetics at undreamed-of pace. Computational screening and data mining allows to explore these data bases for promising materials and extract correlations like structure-property relationships.

At present, these efforts are still largely based on highly reductionist models that break down the complex interdependencies of working catalysts and energy conversion systems into a tractable number of so-called descriptors, i.e. microscopic parameters that are believed to govern the macroscopic function. For certain classes of materials like transition metal catalysts, corresponding human-designed models have indeed established trend understanding and spurred a targeted materials design.

Future efforts will concentrate on using artificial intelligence also in the actual generation and reinforced improvement of the reductionist models. This is expected to better capture complexities like incomplete understanding or operando changes of interfacial morphology, to provide access to structured and compound materials classes, or ultimately to even fulfill the dream of an inverse (de novo) design from function to structure.

In this talk, I will briefly survey these developments, providing examples from our own research, in particular on adsorption energetics at bimetallic catalysts and data mining for the design of organic semiconductors.