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Knowledge-Based Approaches in Catalysis and Energy Modelling (30 min talk + 15 min discussion)

Thursday, 15 April 2021 14:00 (45 minutes)

Data sciences 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 devices into a tractable number of so-called descriptors, i.e. microscopic parameters that are believed to govern the macroscopic function. Generally, static predefined databases are also the norm. Future efforts will concentrate on using artificial intelligence also in the actual generation and reinforced improvement of the reductionist models, and in devising active learning approaches that generate the truly required data on demand. In this talk, I will briefly survey these developments, providing examples from our own research, in particular on data-efficient approaches to reaction kinetics and active machine learning for the design of organic semiconductors.

Poster title

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