CatLab – Putting calculation before experiment in organometallic catalysis

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Computational studies of homogeneous catalysis play an increasingly important role in furthering (and changing) our understanding of catalytic cycles and can help to guide the discovery and evaluation of new catalysts [1, 2]. While a truly "rational design" process remains out of reach, detailed mechanistic information from both experiment and computation can be combined successfully with suitable parameters characterising catalysts [3] and substrates to predict outcomes and guide screening [4].

The computational inputs to this process rely on large databases of parameters characterising ligand and complex properties in a range of different environments [5-8]. Such maps of catalyst space can be combined with experimental or calculated response data [7], as well as large-scale data analysis. Rather than pursuing a purely computational solution of *in silico* catalyst design and evaluation, an iterative process of mechanistic study, data analysis, prediction and experimentation can accommodate complicated mechanistic manifolds and lead to useful predictions for the discovery and design of suitable catalysts. In this presentation, I will use examples drawn from our recent work, including the early stages of our development of a reactivity database, to illustrate this approach.

Website: https://feygroupchem.wordpress.com/

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