

Discovery Informatics: A Model-Based Approach to Catalyst Design

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A chemical kinetic model, although an essential ingredient of the understanding of catalytic behavior, does not contain sufficient knowledge to predict improved catalysts. The inherent chemistry of families of catalysts governs relationships between the various rate and equilibrium constants and thus provides the key to the optimal catalyst formulation. We call our strategy at Purdue for identifying and utilizing such information *Discovery Informatics*. This approach to catalyst design envisions building a quantitative *forward model* that links *descriptors* of the catalyst chemistry, through a microkinetic model, to catalyst performance. While such a model has intrinsic value, that value will be powerfully leveraged if the model can be used to predict performance of new materials chosen in a guided stochastic search of the descriptor space. In principle, comparison of the measured performance of the “fittest” materials chosen in that *inverse search* then provides direction for model improvement. Iteration of the prediction- measurement-correction cycle would produce evolution toward an optimal catalyst. In this process, the forward model becomes the repository for catalytic knowledge extracted from the experiments.

Progress in developing this approach will be illustrated with two examples: homogeneous single site olefin polymerization catalysis and heterogeneous water gas shift (WGS) catalysis. In the first case, aryloxide and Cp(Cp^{*}) ligated Ti and Zr catalysts present well defined catalytic sites and a team of researchers has combined DFT computation with kinetic experiments to produce a detailed model that correlates the 1-hexene propagation rate with ion pair separation energies and the cone angles available for monomer docking. Extensions to other systems have been enabled by a population balance kinetic model that can use molecular weight distribution data to fit additional kinetic parameters. Heterogeneous catalyst systems add to the complexity of the design problem because of the many potential catalytic sites often available. Recent literature has shown remarkable success using scaling laws and Brønsted-Evans-Polyani relations to identify optimal catalysts for structure insensitive (facile) reactions. Our work with supported Pt, Pd and Au WGS catalysts shows substantial effects of support, alloying and particle size for this reaction. This system reveals the critical role that experiments, carried out at a fast but precise pace, must serve to help narrow the focus for theoretical analysis and illustrates the need for “scalable” theories to account for the structural details of catalytic sites.