

Predictive Modeling for Catalyst Design

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Catalyst design is an important part of energy production and emissions treatment. The design process involves repetitive experimentation, varying the molecular structures and compositions of the catalyst. Computational methods can then be used to collate the data and build a kinetic model. Though often successful, this is expensive due to the high cost of each experiment. By advancing computational methods to *predict* the detailed reaction kinetics, the number of experiments may be reduced. We can currently predict some reaction systems using an automatic Reaction Mechanism Generator (RMG). This open-source software uses correlations to estimate reaction data. It requires prior knowledge (experimental data) to make these correlations, but in cases where such data are unavailable we need to develop another method to generate the reaction mechanism. We can do this by initializing and tracking the three-dimensional geometry of the reactants and transition states, then finding and optimizing their electronic energies via quantum chemical calculations. Performing these calculations automatically will enable RMG to predict more reaction systems, by expanding its capabilities beyond the existing reaction database.