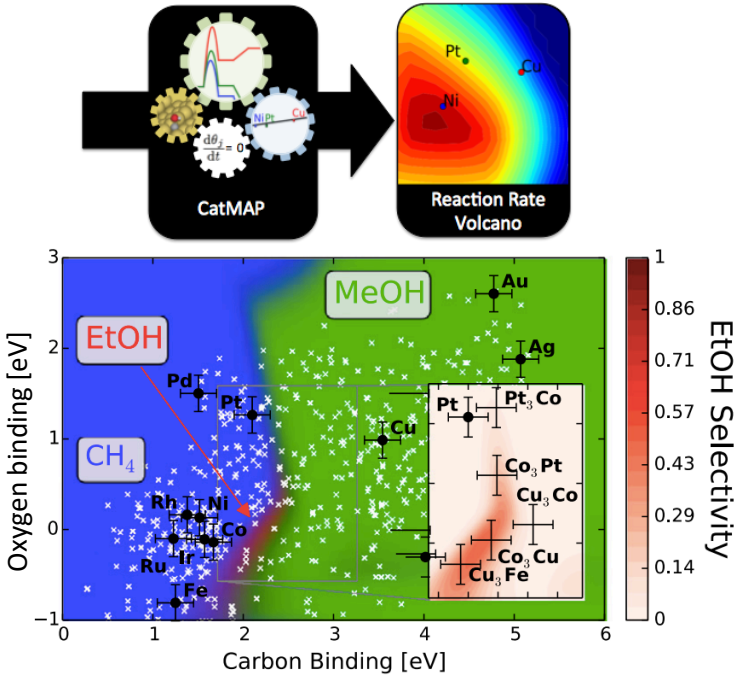
High-throughput Computational Catalyst Screening

Andrew J. Medford, School of Chemical & Biomolecular Engineering

Objectives: Utilize CatMAP software platform to establish correlations between "descriptor" adsorption energies and all relevant intermediate and transition-state energies and integrate the resulting models with micro-kinetic models to map catalytic activity and selectivity trends. This high-thoughput strategy has been tested for academic catalyst design, but the objective of this work is to couple it with an industrial catalyst discovery process.

Concept Illustration:



Technical Approach: The following strategy will be pursued:

- Identify a suitable reaction of interest and a class of possible catalyst materials.
- Leverage existing calculations of adsorption energies and transition-states, along with new DFT calculations, to establish the reaction energetics for a set of representative catalysts.
- Utilize a combination of linear correlations and more advanced machine-learning methods to determine "descriptors" for predicting reaction energies.
- Utilize the CatMAP software platform, originally developed by Medford, to map out the catalytic activity and/or selectivity as a function of descriptors.
- Compute descriptors for thousands of candidate materials using DFT and use the results to recommend novel material compositions for catalyst testing.

Impact: The descriptor-based screening approach has proven successful for numerous test reactions including ammonia synthesis, CO oxidation, and syngas conversion in recent academic studies. However, the technique has not been applied in the context of an industrial catalyst discovery setting. The impact of this project is to identify and address challenges with integrating computational high-throughput catalyst discovery approaches with the realities of industrial catalyst design. This will provide new software tools to accelerate the industrial catalyst design process.