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["Towards Accurate Mechanistic Models of Catalytic Systems using Data-driven Techniques"](#)

Abstract: Nearly a trillion dollars-worth of chemical products (petrochemicals, agrochemicals, specialty chemicals, etc.) require a catalyst for their synthesis. Consequently, there is great interest in rationally designing new catalysts that are more efficient (from both energy and material standpoints) than the current ones. The first step towards this is to develop a fundamental mechanistic understanding of the catalytic system. Using a combination of ab initio calculations, experimental thermokinetics data, and a variety of data-driven techniques such as multi-fidelity modeling, surrogate modeling, and Bayesian inference, we demonstrate a modeling framework that allows one to build detailed and accurate models of catalytic systems, using examples from the field of heterogeneous catalysis.