

Audacity of huge: machine learning for the discovery of transition metal catalysts and materials

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I will discuss our efforts to use machine learning (ML) to accelerate the computational tailoring and design of transition metal complexes and metal-organic framework (MOF) materials. One limitation in a challenging materials space such as open shell, 3d transition metal chemistry is that ML models and ML-accelerated high-throughput screening traditionally rely on density functional theory (DFT) for data generation, but DFT is both computationally demanding and prone to errors that limit its accuracy in predicting new materials. I will describe three ways we've overcome these limitations: i) through efficient global optimization to minimize the numbers of calculations carried out to obtain design rules in weeks instead of decades while satisfying multiple objectives; ii) through machine-learned consensus from a family of dozens of functionals to more robustly uncover new materials; and iii) by the use of natural language processing to extract, learn, and directly predict experimental measures of stability on heterogeneous MOF materials.