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"Using Machine Learning and First-Principles Simulation to Automate the Design of Transition Metal Complexes."

Abstract: We will review advances made in the Kulik group towards the virtual design of transition metal complexes using a hybrid density functional theory (DFT) simulation and machine learning (ML) approach. Using information from the molecular graph only, we train artificial neural networks (ANNs) to predict spin state ordering, equilibrium bond lengths, orbital properties and catalytic energies based on DFT references. We combine these predictive surrogate models with novel uncertainty metrics and algorithmic developments to efficiently and accurately search large, unexplored design spaces for complexes with targeted properties. We further show how ML methods can enhance structure generation, optimize workflow control by avoiding fruitless calculations and estimate sensitivity to functional choice.