Expanding Methods from Computationally-Driven Design of Catalysts to Designing Advanced Materials

*Zhu, J.[1] and Getman, R. B.[2]
[1]Graduate Research Assistant, Department of Chemical and Biomolecular Engineering, Clemson University, jiazhoz@g.clemson.edu
[2]Associate Professor, Department of Chemical and Biomolecular Engineering, Clemson University, rgetman@g.clemson.edu

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In this work, we expand methods from computationally-driven design of catalysts to designing substituted metal ferrites for applications in magnetically modulated energy delivery (MagMED). Specifically, computational catalysis involves using density functional theory (DFT) to calculate thermodynamic and kinetic quantities of chemical reactions as they occur over a handful of catalysts, i.e., materials that increase the rates of chemical reactions without being consumed, themselves. The thermodynamic and kinetic quantities are analyzed statistically in order to identify one or two "descriptors". These descriptor quantities are well-correlated to all of the other thermodynamic and kinetic quantities and are used to construct "scaling relationships," which are linear equations that take the descriptors as independent variables and produce as dependent variables estimates of the remaining thermodynamic and kinetic quantities. The scaling relationships are input to a microkinetic model, which combines the thermodynamic and kinetic quantities with models from statistical thermodynamics, in order to construct rate equations for the elementary steps. These are coupled with reactor design equations to produce a system of equations, which, when solved yields information about the catalytic rate. In computational catalyst design, the goal is to identify the optimal descriptor values, which maximize the rate and/or selectivity of the desired product. The material properties that control these optimal descriptor values can then be sought using a machine learning regression procedure. In this poster, we demonstrate the use of computationally-driven catalyst design of transition metal nanoparticle catalysts for n-butane selective oxidation to 1-butanol. We identify catalytic descriptors that optimize activity and selectivity for this reaction. Then, we discuss how machine learning can be used to determine the material and electronic properties (e.g., electronegativity, HOMO-LUMO gap) that dictate the descriptor values. Knowing this information aids in materials selection. Finally, we discuss our initial efforts at applying these same methods to identifying the correlation between composition and magnetic properties, specifically the magnetic moment and anisotropy, of substituted metal ferrites. The ultimate goal of this project is to learn how to tune the magnetic properties of substituted metal ferrites by altering their compositions. Ultimately, these rationally-designed MagMED materials will be applied to treating disease.