Computationally-Guided Design of Materials: From Garnering Fundamental Understanding to Optimizing Material Performance

Jiazhou Zhu and *Rachel B. Getman
PhD Candidate, Clemson University and Associate Professor, Clemson University

Presentation Keywords: quantum calculations, kinetic modeling, machine learning, catalysts, substituted metal ferrites

At the heart of the Materials Genome Initiative (MGI) is the integration of computation, simulation, digital information, and experimentation. Computationally-driven design uses each of these to at least some degree, with the aim being to learn how materials function for particular applications. A key objective is to identify the particular material properties that are related to material function, and to tune those properties in order to optimize material performance. In this presentation, we discuss how we have used a combination of quantum mechanics calculations, kinetic modeling, and statistical analysis including machine learning to drive the design of two classes of materials. Specifically, we discuss the design of catalysts for production of fine chemicals and magnetic nanoparticles for development of electronic devices. We demonstrate how we have used computational techniques to identify the properties of these materials that are related to their performances and demonstrate how this knowledge significantly reduces the time required to screen the performances of new potential materials. The next step in each of our projects is to work with our experimental collaborators to bring the optimized materials to fruition. While our studies have led to new insights about how materials function and which properties need to be tuned to optimize their performances, bridging the gap between simulations and synthesis/development/implementation remains a challenge. We discuss some of the challenges in this regard related to our projects and conclude with an outlook addressing some of the outstanding issues in computationally-driven materials design.