Computational Modeling of Renewable Energy

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The overarching goal of our group is to develop new methods to extract sustainable fuels and chemicals from plants. Our approach has been to develop and apply computational tools to both biological and chemical conversion processes as part of an iterative 'model-validate-predict' design process for de novo catalysts.
With its high carbon and hydrogen content, lignocellulosic biomass presents an alternative to petroleum as a nearly carbon-neutral precursor to upgraded liquid fuels. I will present some representative results in designing new catalysts for biological and chemocatalytic processes of biomass.
Our group has introduced a "Fuel property first" design approach to reduce emissions and increase performance. Traditional approaches for developing these mechanistic models require many years for each new molecule, a pace that is poorly suited to the large-scale search for new bioderived blendstocks. We have developed a quantitative structure-property relationship (QSPR) model for sooting tendency based on the experimental yield sooting index (YSI), developed by collaborators at Yale (Prof. L. Pfefferle and Dr. C. McEnally). This is the first fuel property predictive tool using ML (Machine Learning) approaches in combustion research. We have started to build kinetic mechanisms of soot precursor formation during combustion using DFT and flow reactor experiments (collaboration with Dr. R. McCormick, NREL) to show how the fundamental chemistry affects this practical engineering problem..

Seonah completed an MS in Computer Science at the University of Houston with B. Montgomery Pettitt in 2003 and obtained her Ph.D. with Adrian Roitberg at the University of Florida in 2007 in protein simulation. In 2008 she joined the group of K. N. Houk at the University of California, Los Angeles, as a postdoctoral research associate working on de novo enzyme design using a combination of quantum chemistry and classical simulation techniques. In 2011, Seonah joined the National Renewable Energy Laboratory (NREL), where she remains as a senior scientist in the Biosciences Center until 2020. Seonah is experienced in using computation to understand and design catalysts in biotechnology. Mechanisms of various catalysts, both biological and inorganic, have been explored in biochemical and thermochemical conversion processes. Seonah has expanded her research area to consider the reaction mechanisms involved in combustion, the kinetics of autoignition and soot formation, and the development of a fuel property prediction tool using machine-learning and quantum chemistry. She sits on the organizing committee of the American Chemical Society Computers in Chemistry (COMP) Division since 2015 and served as Chair position in COMP Division in 2020. In January 2021, she moved to join the Chemistry department at Colorado State University as an associate professor to start a new scientific journey.