problems in molecular design (both macro and molecular scale), catalysis, organic/inorganic membranes for gas mixture separation, chemical vapor deposition (CVD) and oral drug delivery.

In molecular modeling we have developed a molecular dynamics model of inorganic/organic membranes for separation of gases from a process such as pyrolysis. Specifically, we have studied the separation of CO$_2$/CH$_4$ in collaboration with membrane experimentalists. The idea is to use the MD model to possibly guide better membrane designs.

At a macro level we have made some inroads into the systematic design of compounds with desired physical and/or chemical properties. We refer to such computer-based compounds as “designer” compounds. For example, noting that solvents play a very important role in the processing of compounds, we have used the design approach within an optimization model to study the impact of solvents and solvent blends on the morphology of pharmaceutical compounds such as ibuprofen and on reactions such as the Kolbe Schmitt reaction. The latter is widely used in preparing aromatic hydroxy carboxylic acids that are important intermediates in the synthesis of numerous products, including pharmaceuticals and high-polymeric liquid crystals.

Oral drug dosage and release in the gastrointestinal tract is part of an ongoing effort for the development of personalized medicine. In light of this we have developed a computational strategy for pharmaceutical drug tablet customization, namely designing the dosage form of the tablet based on a desired drug release profile. The latter is inspired by a desired plasma concentration profile (therapeutic effect). Our efforts include the systematic identification of tablet geometry and designs that could give specific desired drug release profiles such as a constant release profile or a pulsatile release profile.

Machine Learning (ML) has been rediscovered since about 2006 and is rapidly becoming ubiquitous in STEM areas including chemical engineering. I will show how we have used ML for catalysis, fuel-cells and in the early identification of autism in very young kids so as to provide timely interventions in their development.

Zinc sulfide has received a significant amount of attention during the last two decades. Compared to other semiconductors, zinc sulfide has a large direct band gap, which makes it useful in a broad range of optical applications. A common cause of defects in the deposited film during CVD is due to the variability in the morphology of adducts in the gas phase and in the deposited film. We have employed molecular dynamics and agent-based strategies to predict the size distribution and morphology of molecular clusters that impact defect formation.