We design and characterize new materials at the nanoscale through the use of theory and computation. Our research focuses include drug design through prediction of physical properties and binding affinities and the design of novel biomimetic materials. We are especially interested in the development of computational tools that can fundamentally change molecular design by making searches through chemical and configurations space much more predictive, reliable, and efficient.

“Developing atomistic simulation of molecular materials in order to create fundamentally new ways to design novel pharmaceutical and other nanoscale products.”