My research is in the area of computer simulations of complex molecular systems, focusing on developing and applying atomistic models to solve interesting chemical and biological problems. Our goals are to relate the detailed microscopic information provided by the simulations to determine observable physical, chemical and biological properties. Besides providing a basic understanding of biologically important molecules, the simulation results yield predictions on how to manipulate the properties for practical purposes, including design of drugs and novel materials.

Student projects in my laboratory involve molecular dynamics simulations of complex systems as part of ongoing research: folding and function of peptides and small proteins, permeation of peptides through biological membranes, analysis of behavior of disordered proteins, and correlating molecular motions with observed spectroscopic signals. Prof. Kuczera has two papers published with undergraduate students.

