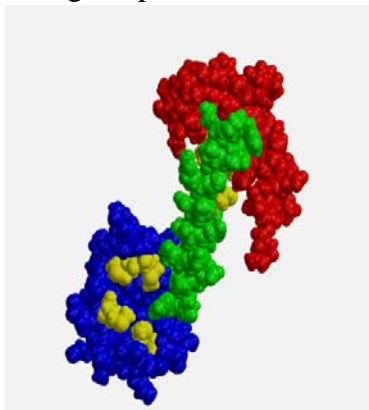


Krzysztof Kuczera, Computational chemistry and biochemistry

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 provide 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. These projects range from predictions of transport properties of novel liquid media for chemical processing, correlations between simulated atomic details of peptide motions with observed spectroscopic signals and descriptions of protein-protein and protein-DNA interactions involved in metabolic regulation. Prof. Kuczera has two papers published with undergraduate students.

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