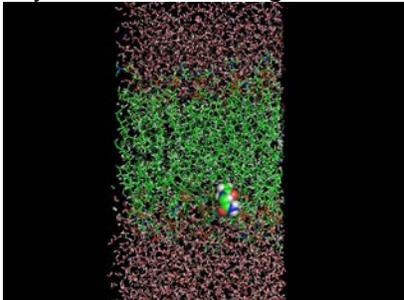


Computational Chemistry and Biochemistry

Prof. Krzysztof Kuczera

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: response of peptide structure and dynamics to changes in environment – including temperature, pH, external forces, stabilizing and destabilizing co-solvents and presence of membranes, as well as correlating molecular motions with observed spectroscopic signals. Prof. Kuczera has two papers published with undergraduate students.

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