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 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 molecular motions with observed spectroscopic signals, thermodynamic and kinetic description of transmembrane transport, and modeling of structure, dynamics, interactions and function of peptides and proteins. Prof. Kuczera has two papers published with undergraduate students.

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J. Unruh, K. Kuczera and C.K. Johnson, "Conformational Heterogeneity of a Leucine Enkephalin Analog in Aqueous Solution and SDS Micelles: Comparison of Time-Resolved FRET and Molecular Dynamics Simulations", *J.Phys.Chem. B,* **113:**14381-14392 (2009).

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