Physics Colloquium

"The Extraordinary Fluctuating Electrostatic Landscape of Proteins and Water as seen through Newtonian Dynamics + Quantum Mechanical Simulations of Fluorescence Wavelengths and Intensity."

Professor Patrik Callis
Department of Chemistry & Biochemistry
Montana State University

Friday, December 7, 2012
4:10 – 5:00 pm, EPS108

Abstract: Living organisms (including humans) employ tens of thousands of precisely folded proteins to perform specific tasks necessary for the process called living. Thousands of scientists studying proteins rely on the intensity and wavelength of emitted light (fluorescence) from the amino acid tryptophan (Trp) because it is extremely sensitive to its "environment" in a protein. This means in practice that any structural change in a protein during its function will cause a change in intensity/wavelength. As of 2002, what was meant by "environment" was completely mysterious. Not one person on the planet could examine a crystal structure of a protein showing in detail the atoms near a Trp and determine whether it would emit with high or low efficiency. In the last several years, we have combined classical molecular dynamics with simplified quantum mechanics to gain considerable predictive power. Our success came from placing more emphasis on the density of states (i.e. resonance and fluctuations) instead of the more "popular" electronic coupling part of Fermi's golden rule as applied to quenching of fluorescence by electron transfer to the protein backbone amides.

Host: Rufus Cone

Refreshments 3:45 p.m.
EPS 2nd Floor Atrium