



Friday, November 15, RUN auditorium, 2:00 PM

Complexity with a purpose: Long range collective vibrations steering protein conformational change

The evolutionary advantage of the large-scale structure of proteins surrounding the biochemically active site is not readily apparent. It has been speculated that the structural dynamics provide long-range control of access to the active site. Through anisotropic terahertz micro-spectroscopy (ATM) measurements we find that the photo initiation of orange carotenoid protein's (OCP) photocycle is accompanied with switching in the protein structural vibrations, before long range structural change can occur. The ATM spectral changes are reversible and calculations reproduce the changes in ATM spectra, with features red shifted from the measurements. Averaging the vibrational displacement autocorrelation matrix over the spectrally relevant region and thermally occupied starting configurations finds changes in the correlations for residues 80-113 with residues 151-164, and for residues 280-291 with residues 265-275. These regions are those previously predicted to be involved in the structural modification necessary for a critical step in the photocycle. The results provide the first evidence that structural vibrational change can actuate conformational change for function.



Prof. Dr. Andrea Markelz

Department of Physics
University at Buffalo, SUNY

Host: Rupert Huber