

Kemijski inštitut Ljubljana Slovenija

National Institute of Chemistry Slovenia

http://www.ki.si

VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

Prof. Dr. Andrea Markelz

Department of Physics, University at Buffalo, SUNY, 239 Fronczak Hall, Buffalo, New York, 14260, USA, e-mail: amarkelz@buffalo.edu

Ponedeljek, Monday, 26. 5. 2014, ob / at 10:30

Velika predavalnica Kemijskega inštituta / Lecture Hall at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

MEASUREMENTS OF LONG-RANGE PROTEIN MOTIONS

Allosteric control of enzymatic reactions continues to be a field of interest as an avenue of species specific drug design that targets critical pathway enzymes. A natural question is why the remote regions of protein are correlated to the substrate site? A particular compelling mechanism is collective vibrational motions of the protein, which involved correlated motion both at the remote site and the binding site. If these long range motions specifically access binding configurations then allosteric control is a natural consequence of perturbing the long range motion at the remote site. Direct measurements of collective modes previously involved either X-ray or neutron scattering, limiting the measurements undertaken. Here we discuss measurements of the frequency and structural dependence of collective modes using crystal anisotropy terahertz microscopy (CATM) [1]. This new technique removes the strong isotropic relaxational background from librational motions of the solvent and surface side chains. In addition, anisotropy measurements have the potential to aid in mode identification, as we found previously for molecular crystals. For large systems such as proteins we need to consider general groups of motions. In particular the anisotropy indicates the general structural dependence of accessible motions. We consider methods to distil the dense density of states and isotropic spectrum to spectral regions specifically associated with motions that are spectrally relevant.

[1] Acbas, G., K.A. Niessen, E.H. Snell, and A.G. Markelz, *Optical measurements of long-range protein vibrations.* Nat Commun, 2014. **5**.

Vljudno vabljeni! / Kindly invited!

info: dr. Franci Merzel; franci.merzel@ki.si