Ultrafast 2D IR Spectroscopy as a Structural and Dynamical Probe of Biomolecules: From Enzyme Active Sites to Non-Canonical Nucleic Acid Motifs – and Beyond

Dr. Sean D. Moran

Assistant professor

School of Chemical and Biomolecular Sciences

Southern Illinois University Carbondale

Chemistry Seminar on *Ultrafast 2D IR Spectroscopy*

Monday Oct. 9 at 4 pm in 303 Schrenk

Please contact Dr. Amitava Choudhury at choudhurya@mst.edu for further information.

MISSOURI S&T

Abstract: Ultrafast two-dimensional infrared (2D IR) spectroscopy is a sensitive probe of molecular interactions and motions in condensed phases, and my group leverages several of its advantages to study biomolecular phenomena that are largely 'out of reach' to other experimental techniques. In this talk, I will introduce the method and highlight how we apply it in various areas of research. First, I will discuss how we use 2D IR and site-specific vibrational labels to examine femtosecond-picosecond timescale fluctuations in enzymes bound to substrate (or inhibitor) analogs. By engineering molecular structures, we gain detailed insight into how ultrafast phenomena vary with position and orientation in the active sites of two enzymes: a hyperthermophilic archaeal ene-reductase and the human lysine methyltransferase SET7/9. Second, I will discuss how we use vibrational coupling and metal-dependent frequency effects to deduce the structures of DNA G-quadruplexes with infrared spectroscopy. Third, I will introduce our exploratory work on protein aggregation among members of the Bcl-2 family, which are critical in programmed cell death (apoptosis) and are involved in many human diseases.

About the speaker: Sean Moran received his Ph.D. from Columbia University in 2008, where he worked with Prof. Brian Gibney on *de novo* design of model redox proteins and mononuclear metalloproteins. In 2009, he joined Prof. Martin Zanni's group (University of Wisconsin-Madison) as a postdoc, where he applied ultrafast 2D IR spectroscopy and heavy isotope labeling to examine the aggregation of cataract-forming eye-lens proteins as well as potassium binding to the selectivity filter of a bacterial K^+ channel. In 2014, he joined the School of Chemical and Biomolecular Sciences at Southern Illinois University Carbondale as an Assistant Professor. His group's research uses 2D IR spectroscopy to address problems in protein misfolding, the formation of non-canonical nucleic acid structures, and the connections between enzyme dynamics and function.