

# Physical Chemistry Seminar

Tuesday,  
April 14, 2015

11:00 am

Room 1315  
Chemistry Building

## Gaining Insights into Nanoaggregate Structures of Polycyclic Aromatic Hydrocarbons with 2D IR spectroscopy



Professor Amber Krummel

*Department of Chemistry  
Colorado State University*

*Host: Professor Marty Zanni*

Polycyclic aromatic hydrocarbons (PAHs) are broadly used to construct supramolecular nanomaterials and occur naturally in our environment in the form of humic acids and asphaltenes, for example. Solvent dynamics and intermolecular interactions including  $\pi$ -stacking, play integral roles in the self-assembly of these molecules. In this talk, I will discuss our work using 2D IR spectroscopy to probe the intermolecular interactions that are prevalent in self-assembled PAH molecules. A model PAH is investigated—violanthrone-79. Violanthrone-79 has strong carbonyl oscillators as part of the PAH conjugated ring systems and are used here to report on the intra- and intermolecular interactions in self-assembled PAHs. However, the carbonyl and ring vibrational motions are mixed in the vibrational eigenstates that lie between  $1550\text{ cm}^{-1}$  and  $1720\text{ cm}^{-1}$ . In order to better understand the nature of the vibrational eigenstates in these PAH molecules, we include a systematic investigation of a series of small aromatic ketones and quinones with one, two, and three rings.<sup>1</sup> We have found that the vibrational coupling in these molecules spans the strong to weak coupling limits depending upon the number of rings in the molecule. These investigations are used to develop a model that quantitatively describes the vibrational coupling in the violanthrone-79. Ultimately we use our models to determine the PAH aggregate structure by simulating the 2D IR spectra based on the foundations set in our small molecule investigations.<sup>2</sup>

1. Cyran, J.D., Nite, J.M., and Krummel, A.T. **Characterizing Anharmonic Vibrational Modes of Quinones with Two Dimensional Infrared Spectroscopy**, *Journal of Physical Chemistry, B*, 2014, DOI: 10.1021/jp506900n.

2. Cyran, J.D. and Krummel, A.T. **Probing Structural Features of Self-Assembled Violanthrone-79 using Two-Dimensional Infrared Spectroscopy**, *Journal of Chemical Physics*, 2015, submitted.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8305F