ANALYTICAL SEMINAR

Understanding Interfacial Chirality: Dark-Field Absorbance Circular Dichroism of Oriented Chiral Thin Films

Gwendylan Turner

Graduate Student
Purdue University

Abstract: Chirality exhibits our universe on all length scales: from the behavior of sub-atomic particles to galaxies. Molecular and supramolecular chirality play critical roles in the formation and interactions of various systems and are accessed experimentally through chiroptical spectroscopies. While molecular chiroptic responses of isotropic systems are regularly studied and well-understood, responses of uniaxial systems remain clouded despite their natural ubiquity and importance, particularly to interfacial systems. Herein, a theoretical framework is proposed to predict the chiral-specific responses of uniaxially oriented systems, revealing that nonreciprocal circular dichroism (CD) can arise purely within the electric dipole approximation and can be connected back to molecular structure and orientation. The model accurately predicts the magnitude, sign, and orientation-dependent behavior of a benchmark system without adjustable parameters. Additionally, the association of depolarization of the transmitted beam with the anisotropic response is central to the proposed framework, and this connection is further validated through the design and implementation of dark-field and confocal approaches to CD spectroscopy.

Bio: Gwendylan is a PhD candidate in the Garth Simpson Group at Purdue University, where she has worked to develop and improve spectroscopic techniques with physics-based approaches. She currently fosters a collaboration between Purdue and Lawrence Berkely National Laboratory through a research assistantship on fluorescence-detected photothermal infrared spectroscopy. Prior to Purdue, Gwendylan obtained her B.S. in Chemistry from the College of William and Mary, where she used gas-phase ion-ion reactions to inform on how post translational modifications affect the thermodynamic properties of amino acids. She is a recent recipient of Purdue's Guy Mellon Award in Analytical Chemistry and of the Eastman/ACS Analytical Chemistry Fellowship.

Tuesday, April 29, 2025 | **3:30 pm** | **WTHR 320**

PURDUE UNIVERSITY
James Tarpo Jr. and Margaret Tarpo Department of Chemistry

ANALYTICAL SEMINAR

Identification of the Aromatic Aldehyde and Keto Functionality in Protonated Polyfunctional Analytes via Gas-phase Ion-molecule Reactions Followed by Collision-activated Dissociation in a Linear Quadrupole Ion Trap Mass Spectrometer

Jaskiran Kaur

Graduate Student
Purdue University

Abstract: The detection and identification of potentially mutagenic drug impurities and metabolites, such as aldehydes and ketones, is of utmost importance for the pharmaceutical sector. Therefore, it is critically important to develop analytical techniques that enable their unambiguous identification. The use of tandem mass spectrometry (MS/MS) based on collision-activated dissociation (CAD) of analyte ions is a commonly employed technique for identifying unknown organic substances within complex mixtures. However, CAD often produces similar patterns of fragmentation for isomeric ions, making it challenging to identify or even distinguish these ions. Furthermore, CAD can cause isomerization of the ionized analytes prior to or during fragmentation. To address these limitations, diagnostic gas-phase ion-molecule reactions of protonated analyte molecules can be employed to differentiate isomeric ions and identify specific functional groups in protonated analytes. This seminar will cover the method development for the identification of analytes with aromatic aldehyde and keto functionalities via diagnostic gas-phase ion-molecule reactions of trimethoxymethylsilane with the protonated polyfunctional analytes followed by CAD experiments by using a linear quadrupole ion trap mass spectrometer. Quantum chemical calculations were employed to elucidate the mechanisms of the relevant reactions.

Bio: Jaskiran is a fourth-year graduate student in the Kenttamaa Group. She earned her M.S. and B.S. degree in Organic Chemistry from Hindu College, University of Delhi, India. Her research interests include studying mass spectrometric ion-molecule reactions and gas-phase reactivities of boron radical anions. She has contributed to several projects aimed at advancing analytical methods and promoting interdisciplinary collaboration. She is the recipient of the Robert R. Squires Scholarship (2024) for high-impact research in physical organic chemistry and the Thomas W. Keough Graduate Scholarship (2025) for excellence in mass spectrometry and teamwork.

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