WORKSHOP # 4 – Wednesday, April 22, 2026

Non-Conventional Infrared Spectroscopy and Imaging

Organizers:
Anibal Boscoboinik (CFN, BNL), Lukas Wehmeier (NSLS-II, BNL), Sabrina Gericke (CFN, BNL), Maya Endoh (Stony Brook University)

Infrared (IR) spectroscopy is a cornerstone technique for probing molecular structure, bonding, and chemical composition across a wide range of scientific disciplines. By directly probing vibrational modes, IR spectroscopy provides chemically specific insight into functional groups, local environments, and dynamic processes that underpin behavior in complex systems. IR spectroscopy is widely used in semiconductor and nanomaterials characterization, microelectronics and photonic device development, polymer and soft matter science, catalysis, membrane biophysics, and studies of chemical and biological interfaces. In quantum materials, infrared techniques play a critical role in elucidating electron–phonon coupling, lattice dynamics, and emergent excitations that influence electronic and optical properties.

Although these applications span diverse disciplines, many share common experimental challenges, including chemical heterogeneity, buried interfaces, and the need to probe materials under realistic conditions. Increasingly, IR methods are implemented under in situ and operando environments, enabling researchers to follow chemical reactions, phase transformations, and interfacial processes in real time under reactive gases, liquids, electrochemical potentials, or applied thermal and mechanical stimuli.

Recent advances have significantly expanded the scope of infrared spectroscopy and imaging beyond conventional far-field measurements. Emerging and non-traditional IR approaches now enable enhanced surface and interface sensitivity, nanoscale spatial resolution, and access to heterogeneous or buried structures. Near-field and photothermal methods overcome diffraction limits and allow chemically specific imaging with nanometer-scale resolution, while nonlinear and interface-selective IR techniques provide molecular-level insight into interfacial structure and chemistry.

This workshop aims to introduce users from a wide range of scientific backgrounds to current and emerging infrared spectroscopic and imaging capabilities. The session is designed to be accessible to both experienced spectroscopists and users new to IR methods, emphasizing shared principles, practical considerations, and adaptability across disciplines. These concepts will be illustrated with science examples relevant to materials science, microelectronics, and chemical and biological interfaces. Invited speakers will cover techniques including a general overview, scanning near-field optical microscopy (SNOM), photothermal infrared (PTIR), sum frequency generation (SFG), and infrared reflection absorption spectroscopy (IRRAS). The workshop will conclude with an open discussion about current IR methods available at CFN and NSLS-II, and potential additions of interest to the user community.

Start Time (ET)	Title	Speaker (Affiliation)
12:00 – 2:00 pm	*Lunch Break (travel to/from SUSC to Berkner Hall)*	
2:00	Welcome remarks and NSLS-II and CFN facilities overview	Lukas Wehmeier and Anibal Boscoboinik (BNL)
2:30	An Optical Nanoprobe of Quantum Material Systems	Mengkun Liu (SBU)
3:00	In Situ ATR-FTIR and ML-Driven Spectroscopy for Organic Electrosynthesis: From Electrical Double Layer Probing to Product Analysis	Ricardo Mathison (JHU)
3:30	*Break*	
4:00	Probing the mineralogy and organic speciation of extraterrestrial materials using multimodal micro- and nano-scale spectroscopy.	Timothy Glotch (SBU)
4:30	Probing structure and chemistry at buried interfaces with vibrational sum frequency generation	Ben Doughty (ORNL)
5:00	Atomic Force Microscopy-Based Two-dimensional Infrared (AFM-2DIR) Spectroscopy	Xiaoji Xu (SBU)
5:30	Discussion: Future of CFN and NSLS-II facilities for Non-Conventional Infrared Spectroscopy and Imaging	
6:00	Adjourn	

Abstracts

Mengkun Liu (SBU): An Optical Nanoprobe of Quantum Material Systems

Quantum Hall states and superconductivity are landmark macroscopic quantum phenomena, yet their low-energy spectroscopic structure, nanoscale inhomogeneity, and local coupling mechanisms often remain hidden below the diffraction limit. In this talk, I will present two emerging infrared nanoscopy platforms—magneto-scanning near-field optical microscopy (m-SNOM) and BOlometric Superconducting Optical Nanoscopy (BOSON)—and discuss how they expand non-conventional infrared spectroscopy and imaging for quantum materials. Using m-SNOM, we directly visualize Landau-level-related optical responses and magneto-polariton formation with nanometer-scale resolution, enabling real-space studies of field-tunable light–matter coupling. Using BOSON, we integrate superconducting transition-edge sensors with near-field optics to achieve ultra-sensitive detection of nano-light at sub-nanowatt power, opening a path toward quantum-limited nanospectroscopy in superconducting and strongly correlated systems. I will also highlight AI/ML-enabled measurement strategies, including adaptive scan control, feature-guided spectroscopy, and accelerated analysis of high-dimensional datasets, which improve efficiency and discovery potential. Together, these advances point toward AI-assisted infrared nano-imaging workflows that can complement and extend future synchrotron beamline capabilities, including planned near-field developments at BNL INF.

Ricardo Mathison (JHU): In Situ ATR-FTIR and ML-Driven Spectroscopy for Organic Electrosynthesis: From Electrical Double Layer Probing to Product Analysis
In this work, we designed and fabricated an electrochemical flow cell integrated with in situ ATR-FTIR spectroscopy to probe the electrical double layer (EDL) during acrylonitrile electrohydrodimerization to adiponitrile (ADN), a key precursor in nylon production. We developed a baseline correction algorithm to deconvolute polarization-induced spectral shifts and enable reliable spectral comparisons across varying applied currents. Our measurements reveal that tetraalkylammonium ions populate the EDL at cathodic potentials, enhancing the local concentration of the reactant while expelling water molecules in a size-dependent manner that promotes selectivity toward ADN. Complementing these near-electrode insights, we developed a supervised machine learning framework trained on low-field benchtop NMR spectra to classify and quantify chemicals relevant to nylon precursor synthesis, achieving ~95% classification accuracy and quantification errors near the instrument detection limit.

Timothy Glotch - Geoscience (SBU): Probing the mineralogy and organic speciation of extraterrestrial materials using multimodal micro- and nano-scale spectroscopy.
Recent advances in synchrotron and laboratory instrumentation and techniques have enabled micron and sub-micron spectroscopic analyses of the mineralogy and organic speciation of extraterrestrial materials including meteorites, Apollo lunar samples, and returned samples from asteroids Ryugu and Bennu. We use infrared spectral imaging to probe the mineralogy of fine-grained lunar regolith breccias and to identify and characterize anomalously silicic clasts in the samples. The infrared spectral properties of these clasts are similar to those of lunar silicic volcanic domes and plutons exposed by impact craters. Returned carbonaceous asteroid samples are micro- and nano-breccias that are heterogeneous at every spatial scale investigated. Nano-infrared spectroscopy provides 20-nm scale resolution of fine-grained matrix silicate, carbonate, and phosphate mineralogy and organic speciation to provide new insights into the conditions of aqueous alteration on these asteroid parent bodies.

Ben Doughty (ORNL): Probing structure and chemistry at buried interfaces with vibrational sum frequency generation
Interfaces host key interactions underlying phenomena in critical material separations, soft matter electronics and biological function. While the importance of interfaces is well appreciated, there is a surprising lack of insight into how molecular constituents self-assemble into emergent interfacial structures capable of function. Here, we will discuss recent progress in our labs using surface specific vibrational sum frequency generation to identify functional assemblies and metastable states at buried liquid interfaces that arise from the cumulative interactions of ions, molecules, and materials. This foundational knowledge points to mechanisms by which functionality can be designed into active interfaces using competitive interactions in both phases to alter reactive outcomes.

Xiaoji Xu (Last Speaker) (SBU): Atomic Force Microscopy-Based Two-dimensional Infrared (AFM-2DIR) Spectroscopy
Infrared (IR) spectroscopy has advanced on two distinct frontiers: enhancing spatial resolution and broadening spectroscopic information. While atomic force microscopy (AFM)-based IR microscopy reaches sub-10 nm spatial resolutions, overcoming Abbe's diffraction limit, time-domain two-

dimensional IR spectroscopy (2DIR) provides unparalleled insights into molecular structures, mode coupling, and energy transfers. These two realms, however, evolved in parallel. Here, we will present our work to bridge their boundary. We introduce the AFM-2DIR nano-spectroscopy that offers the spatial precision of AFM with the rich spectroscopic information of 2DIR. This innovative approach utilizes the mechanical detection of the sample's photothermal responses from a tip-enhanced femtosecond IR pulse sequence. We demonstrate it on the carbonyl mode, revealing its anharmonicity. Furthermore, utilizing the tight tip enhancement, we photothermally probe hyperbolic phonon polaritons in isotope-enriched h-BN. Our measurement reveals energy transfers between phonon polaritons and phonons. The AFM-2DIR nano-spectroscopy enables in situ investigations of vibrational anharmonicity, coupling, and energy transfers in heterogeneous materials and nanostructures, especially suitable for unraveling the relaxation process in nanomaterials in IR frequencies.