



DEPARTMENT OF PHYSICS AND ASTRONOMY

COLLOQUIUM **IN-PERSON ONLY EVENT**



PAHsing to Compute Vibrational Spectra in the Age of JWST

Ryan Clifton Fortenberry

*Associate Professor of Chemistry
Graduate Program Coordinator
University of Mississippi*

Recent developments in quantum chemistry are finally allowing the realization of quantum chemical predictions for IR spectra of polycyclic aromatic hydrocarbons (PAHs) which are believed to be the primary IR features observed with the James Webb Space Telescope. While PAHs have been theorized to exist for nearly 40 years now, only recent detections of CN-PAHs (with their large dipole moments) have conclusively shown that they can and do exist in interstellar environments. Even with this conclusive evidence, experimental IR spectra of PAHs are difficult to obtain due to PAHs' propensity for sticking together (creating tar and soot), and the regularity of the various PAH molecules makes separating their behavior nearly impossible. However, quantum chemistry provides the spectra purely from the structure of the molecule, but molecules of this size have been effectively off-limits due to the computational cost until now. This work will highlight how emerging technologies are paving the way for predictions of the fundamental CN stretches in CN-PAHs as well as for how the atomic vibrations within PAHs themselves may be linked to observations from JWST.



Thursday, September 25, at 3:55 PM

IN-PERSON EVENT ROOM 202

Local Contact: Dr. Tho Nguyen, ngtho@uga.edu