Molecular Spectroscopy and Dynamics on Multiple Potential Energy Surfaces

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Chemistry Seminar on *Molecular Spectroscopy*

Thursday April 13 at 4 pm in 303 Schrenk

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Abstract: Research in the University of Louisville Laser labs (UL^3) (https://sites.google.com/site/uofllaserlabs/) consists of spectroscopic studies of gas-phase molecules and condensed-phase materials using state-of-the-art high-resolution and ultrafast laser systems and cutting-edge spectroscopy techniques. Our high-resolution spectroscopy studies center on the detection and characterization of open-shell molecules on multiple potential energy surfaces (PESs). Our target molecules include molecular free radicals as reactive chemical intermediates in combustion and atmospheric chemistry. The spectroscopic methods employed include laser-induced fluorescence/dispersed fluorescence (LIF/DF) spectroscopy for alkoxy (RO·) radicals and cavity ring-down (CRD) spectroscopy for peroxy (ROO·) radicals. These two techniques are also used to study metal-containing molecules, e.g., alkaline-earth monoalkoxide radicals (MORs), which have been proposed as candidates for direct laser cooling and will have important applications in quantum computing, quantum information, and fundamental physics. Recently, our group has built a mid-infrared high-resolution laser spectroscopy apparatus to support the observations of the James-Webb Space Telescope (JWST) and started developing a novel cavity-enhanced double-resonance spectroscopy technique to investigate molecular "dark states" and to decipher the complex energy level structure and intramolecular interactions. On the theoretical side, we are particularly interested in molecular species with the Jahn-Teller (JT) and pseudo-Jahn-Teller (pJT) effects, symmetry-specific vibronic (vibrational-electronic) interactions that cause spontaneous distortion of the geometry and PESs of polyatomic molecules in degenerate or nearly degenerate electronic states. Spectroscopic models and software have been developed to predict, analyze, simulate, and fit vibronic, rotational, and fine structures in high-resolution spectra of open-shell molecules. High-level quantum chemistry calculations are used to help understand the geometry, energy level structure, and dynamics of molecules on multiple PESs.

The nature and strengths of inter-state coupling can also be directly detected in time-resolved spectroscopy, a powerful tool for investigating energy and charge transfer processes. I will use the femtosecond pump-probe transient absorption study of excited-state dynamics of molecule-like ligand-passivated $(CdSe)_{34}$ nanoclusters (d=1.6 nm) to demonstrate the capabilities and limitations of ultrafast spectroscopy in understanding charge carrier dynamics in nanostructures and on their interfaces, which can aid in the design of high-efficiency photovoltaic and light-emitting devices.

About the speaker: Dr. Jinjun Liu is a Professor of Chemistry and Adjunct Professor of Physics at the University of Louisville (UofL). He received his B.S. in Physics with a concentration on Optoelectronics at East China Normal University in 1999. For his Ph.D., Jinjun studied Chemical Physics at the Ohio State University (2001-2007). He developed a zeal for high-resolution laser spectroscopy and theoretical molecular spectroscopy in the research group of Prof. Terry A. Miller and through his collaboration with the late Nobel Laureate Prof. Robert F. Curl. As a postdoc in the research group of Prof. Frederic Merkt at ETH Zurich (2007-2010), Jinjun studied, among other species, few-electron molecules H_2 and He_2 by combining Rydber-state- resolved laser spectroscopy and frequency metrology. After a second postdoc work with Prof. Miller, Dr. Liu became an Assistant Professor of Chemistry and Spectroscopy Theme Leader of the Conn Center for Renewable Energy Research at UofL in January 2012. Prof. Liu is a recipient of the NSF CAREER Award (2015), the Flygare Award of the International Symposium on Molecular Spectroscopy (2017), and the Fundamental Physics Innovation Award of the American Physical Society (APS) and the Gordon and Betty Moore Foundation (2018).