University of Central Florida
Department of Chemistry Seminar Series – Fall Semester 2023
Monday, September 23, Location CB2 105

Who What Where When Why: An Attempt to Understand Uranium Trioxide

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Abstract: Uranium trioxide species are ubiquitous in both front and back-end nuclear fuel cycle processes. This stoichiometry can adopt at least six structural forms and an amorphous phase as a function of the processes used to create it. While numerous reports of UO_3 are available from Manhattan Project era research, only recently has systematic investigation revealed the ways in which optical vibrational (Raman and infrared) spectra of can provide insight into underlying crystal chemistry of this complex family of polymorphs. α- and γ-UO_3 are relatively well studied with respect to their structures and resulting spectroscopic observables. β-, δ-, and ε-UO_3 however, are more exotic and require unique preparation conditions. To this end, we have reviewed and optimized synthetic methods for UO_3 phases, performed density functional theory with density functional perturbation theory calculations and assigned features in the optical vibrational spectra to the structural attributes from which they arise. Our investigation of β-UO_3 involved development of a novel analysis method towards assigning specific vibrational modes to the atomic vibrations from which they originate. In exploring, δ-UO_3, we found unexpected Raman-active vibrational modes, and provide insight into possible structural origins thereof. Finally, we solved the structure of ε-UO_3 from powder X-ray diffraction data and confirm that this is indeed a unique structural modification of uranium trioxide. Our combined efforts have illuminated the unique Raman and infrared spectroscopic signatures of UO_3 polymorphs and demonstrate that rapid, nondestructive optical vibrational spectroscopic measurements can provide insight into fuel cycle processes.

Bio: Dr. Spano completed her B.A. in Earth Science & Chemistry in 2012 from Kean University, and her Ph.D. in Uranium Mineralogy and Nuclear Forensics at the University of Notre Dame in 2017. Her research includes synthesis and structure-property relationships in uranium minerals, development of novel nuclear forensic methods for analysis of uranium phases, optical vibrational spectroscopic, and X-ray diffraction investigations of structure-property relationships of nuclear fuel materials for nuclear nonproliferation. Dr. Spano is actively involved in outreach activities and currently serves as Chair of the Diversity, Equity, and Inclusion Committee for the Mineralogical Society of America, Co-Chair of the Diversity, Equity, Inclusion and Belonging Committee for the Nuclear Science and Technology Division of the American Chemical Society, and Vice President of the East Tennessee Chapter of the American Chemical Society's Women Chemists Committee.