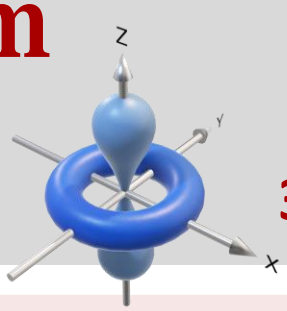
Department of Physics Colloquium

April 25, 2022 **3:00 PM**



A new look at X-ray absorption spectral analysis from a data lens

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X-ray absorption spectroscopy is a premier element-specific experimental technique for materials characterization. Specifically, X-ray absorption near edge structure (XANES) encodes rich local structural and chemical information around X-ray absorbing species, which makes it a powerful tool for probing physical and chemical processes under different experimental conditions. However, the correlation between XANES spectral features and the underlying local structural motifs or electronic descriptors is obscure. Traditional XANES analysis methods rely on prior knowledge of spectral fingerprints of known crystals or first-principles spectral simulations, which have practical limitations on either data availability or computational cost. Here I discuss the recent progress of the field that tackles the problem by leveraging data analytics tools to decipher the structure-spectrum relationship. The utility of this approach is demonstrated in multiple contexts, including extracting physical descriptors [1,2] and developing machine learning models for spectral prediction [3].

1. J. Phys. Chem. Lett., 8, 5091, 2017.
2. Phys. Rev. Mater., 3, 033604, 2019.
3. Phys. Rev. Lett. 124, 156401, 2020.

This colloquium will be held in-person, at SERC 116 unless announced otherwise.