

# DEPARTMENT OF PHYSICS & ASTRONOMY

## Biophysical Seminar

Tuesday, March 27<sup>th</sup>, 2018

3:00 PM, Room 242 Physics  
(Refreshments 2:45 PM)



**Klaus Attenkoefer**

Brookhaven National Laboratory

### From the Spectrum to the Structure — A New Approach in X-ray Spectroscopy

To understand chemical reactions and ultimately to rationally design precursors, substrates, or catalysts, the researcher needs a tool which can image with sub-atomic resolution the structure of the reaction center and its surrounding. This will guide the experimental chemist in making materials with a well defined structure and allows the theorist to baseline his calculations.

Core level spectroscopy, an element selective local probe has the potential to fulfill this role. It is a tool which probes a full ensemble of molecules ensuring representative results, and the local symmetry, hybridization, and structure of the absorber atom. Unfortunately, there is no direct way to extract from the spectrum the structure.

In this talk we will present a new approach in which high-throughput spectroscopy, computation, and database usage are combined to reconstruct the structure of the absorber atom and show how operando or in-situ experiments can be used to understand the structural changes during the processing. Besides the data revealing phase changes during the charging and discharging cycle of batteries and the first attempt to measure a phase diagram of a Zn-Ti-O system, we will provide a background on the experimental and data analysis pipeline which makes this approach possible.

Ultimately, this new tool will be applied to visualize the structural changes during the chemical reaction itself. Ultrafast, highly efficient detection systems will be key to perform these measurements. We will present a new concept which combines ultrathin photocathodes, large area multichannel plates, and pixelated readout electronics which may allow a pulse to pulse separation of 2-4ns, a spatial resolution of 55mm, and a count rate limitation of  $10^{10}$  photons/s. In addition, the time resolution of this system will be discussed which may achieve about 20ps with existing technology but could be pushed into the 100fs regime.