SEMINAR NOTICE

Department of Physics and Engineering Physics
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SPEAKER: Dr. Teak D. Boyko, Senior Scientist REIXS Beamline Responsible
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TOPIC*:* *Determining Crystal Structure using Soft X-ray Spectroscopy*

DATE: Tuesday September 23rd, 2025

TIME: 3:30-4:30 p.m.

PLACE: ***Physics 103***

Abstract:

The continuous discovery new materials have led to the need to develop more complex methods beyond conventional X-ray Diffraction (XRD) to determine the detailed crystal structure. Conventional XRD does not always allow for a complete structural picture given elements of similar atomic numbers can not be distinguished easily, and while neutron diffraction offers an alternative, its lack of availability and the need for large amounts material means it is not always feasible. Contrarily, the electronic structure is very sensitive to the local bonding environments and can be probed effectively using x-ray spectroscopy techniques, which require small amounts of material and also provide elemental selectivity. We combine X-ray Emission Spectroscopy (XES) and X-ray Absorption Spectroscopy (XAS) with Density Functional Theory (DFT) calculations in order to validate a proposed crystal structure by comparing the measured and calculated electronic structure. These tools have allowed us to study more complex crystal structures including the anion ordering of oxygen and nitrogen as well as verifying the presence of structural defects, such as cation vacancies. The general approach to this method, including experimental and theoretical details, and some examples of successfully studies will be presented.