SEMINAR NOTICE

Department of Physics and Engineering Physics
University of Saskatchewan

SPEAKER: Teak Boyko, PhD,
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TOPIC*:* ***Bandgap Engineering of Oxygen-Bearing High-Pressure Zirconium Nitride:*** ***c*-$Zr_{3-x}(N_{1-x}O_x)_4$**

DATE: March 12th, 2019

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

PLACE: Physics 103

ABSTRACT:

Group 4 cubic nitrides, including *c*-TiN and *c*-ZrN, are widely used as refractory materials for coatings on mechanical cutting tools. These materials have been widely studied for their mechanical properties, but very little effort has been spent on ascertaining their electronic properties. More recently, a new structure of cubic group 4 nitrides was discovered, the resulting materials included oxygen bearing *c*-Zr_3N_4 and *c*-Hf_3N_4. There has been extensive research into the electronic properties of this new phase of group 4 nitrides, but few experimental measurements of the electronic band gap exist. Both studies do not conclusively determine the nature of the electronic bandgap and its dependence on the concentration of the oxygen atoms that may be integrated into the structure uniformly. We present measurements of the Local Partial Density of States (LPDOS) for both the O *p*-states and N *p*-states of *c*-TiN, *c*-ZrN, *c*-Zr_3N_4, and *c*-Hf_3N_4 using X-ray Absorption Spectroscopy (XAS) and X-ray Emission Spectroscopy (XES). These measurements are compared to the simulated spectra that were calculated using Density Functional Theory (DFT). From this, the electronic bandgap is measured using the N *p*-states and agrees with the calculated electronic bandgap. Furthermore, the effect of oxygen atoms integrating into the structure of *c*-Zr_3N_4 is explored and alludes to possible bandgap engineering applications.

Coffee and Cookies will be served in Physics lounge at 3:00 p.m. for those attending the seminar.