

# SEMINAR NOTICE

*Department of Physics and Engineering Physics  
University of Saskatchewan*

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**SPEAKER:** Nnanna Ukoji, PhD candidate  
Department of Physics & Engineering Physics

**TOPIC:** *Structure, Electronic Structure and Electronic Spectra of Simple  
Materials at High Pressure*

**DATE:** October 19th, 2021

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

Join Zoom Meeting:

<https://usask-ca.zoom.us/j/96818469630?pwd=aGpiVUtjcEJmZzBqclZ2S042eGpiQT09>

Join by Telephone:

Local Saskatoon Dial-in Number: (639) 638-7474

Other Zoom Dial-in Numbers: <https://usask-ca.zoom.us/j/96818469630>

Join by Video Conferencing Device (SIP):

[96818469630@zoomcrc.com](mailto:96818469630@zoomcrc.com)

Meeting ID: 968 1846 9630

Passcode: 07412447

Telephone Passcode: 07412447

Materials under extreme conditions such as temperature and pressure undergo significant changes in their structure, chemical bonding and properties, which lead to discovery of unusual chemical species not obtainable at ambient conditions. Hence, there is need for an immense understanding of the electronic structure and chemical bonding in these high-pressure materials to interpret the electron sharing, bond formation and nature of bonding formed. In this presentation, I will be discussing the fundamentals of first principles technique including the mostly used density functional theory (DFT) as applied to the interpretation of the unique properties of these materials at high pressure. I will provide an overview of my graduate research including the structure and properties of liquid water and the mechanism of structural phase transition in elemental Cs. The main theme of this presentation is to investigate the validity of the well-established concepts of chemical bonding based on the interactions between localized orbitals on atomic sites. We employed the common bonding analysis methods such as the Natural Bond Orbital Analysis (NBO), Solid State Adaptive Natural Density Partitioning (SSAdNDP), Quantum theory of Atoms in Molecules and the Crystal Orbital Hamiltonian population (COHP) analysis to interpret the electronic structure and bonding of alkali metal transition metal alloys such as K2Ag, K3Ag and the three phases of Na-Au intermetallic. We found that these techniques must be applied with care. The reason being the electron density is modified extensively by pressure, a naive localized description is not appropriate and may lead to erroneous interpretation.