

SEMINAR NOTICE

*Department of Physics and Engineering Physics
University of Saskatchewan*

SPEAKER: Akinpelu Akinwumi, PhD candidate,
Physics and Engineering Physics

TOPIC: *Theoretical Insights into Hydrogen-encapsulated Cage-like Structure and Unveiling the Sodium's Elusive t150 Phase*

DATE: Tuesday January 14th, 2025

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

PLACE: *Physics 103*

Abstract:

The arrangement of atoms in a crystalline structure significantly influences the material's properties. Recently, the discovery of type-VII boron-carbon clathrates, which have calculated superconducting transition temperatures nearing 100 K, has generated keen interest in exploring novel conventional superconductors that can be stabilized at ambient pressure. The electronic structure of these clathrates is highly tunable due to the ability to substitute different metal atoms within the cages, which may also be spacious enough to accommodate small molecules. By integrating molecular hydrogen into a boron-carbon clathrate framework using a first-principles approach, our study reveals a hydrogen-encapsulated clathrate with a superconducting transition temperature of 46 K at ambient pressure. Additionally, by employing a data-driven potential-assisted structure search, we successfully resolve the elusive high-pressure t150 phase of sodium. These findings highlight the unique structural, electronic, and dynamic behaviors of these materials, offering transformative insights into superconductivity and high-pressure physics.

Coffee and Cookies will be available in Phys 177 at 3:00pm for those attending the seminar.