Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **248** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

# Machine Learning-Accelerated Study of Potential Energy Surfaces of Group 14 Elements

*Monday 9 June 2025 15:15 (15 minutes)*

Scientific and technological advancements in numerous areas of physical sciences and engineering rely on the ability to understand and manipulate the properties of matter at the atomic and molecular scale. Density Functional Theory (DFT) excels in approximating the fundamental equations, the Schrödinger equation describing the quantum behaviour of atoms and molecules. Although DFT is considered as the core of continually growing scientific literature, it is prohibitively expensive for simulating large-sized systems requiring long-time scales and is generally limited to moderate sized (a few hundred atoms) systems. While it is essential to follow the principles from the theory, it is important to recognize that the development and modification of simulation algorithms is an art. In this context, to overcome the challenges posed by DFT, this study employs machine learning approaches to accelerate the exploration of the potential energy surface of group 14 elements, both statically and dynamically. This study uses an integrated machine learning-driven metadynamics approach to expedite the investigation of dynamic evolution of phase transitions, grains, and dislocation defects in large Silicon systems under pressure. [1] By using machine learning to accelerate sensible random structure searches, a novel 8H Germanium allotrope with a direct band gap is predicted, positioning it as a promising material for photovoltaic and optoelectronic applications. [2]

References:
[1] Mangladeep Bhullar, Zihao Bai, Akinwumi Akinpelu, Yansun Yao, Phase Transition in Silicon from Machine Learning Informed Meta-dynamics, ChemPhysChem 2024, 25, e202400090.
[2] Mangladeep Bhullar, Akinwumi Akinpelu, Yansun Yao, Unveiling Novel Direct Bandgap Allotropes of Germanium: A Computational Exploration, Computational Materials Today 2024, 2-3, 100009

## Keyword-1

Machine Learning

## Keyword-2

Crystal structure search

## Keyword-3

**Author:** BHULLAR, MANGLADEEP

**Co-authors:** Mr AKINPELU, Akinwumi (University of Saskatchewan); Prof. YAO, Yansun (University of Saskatchewan); Mr BAI, Zihao

**Presenter:** BHULLAR, MANGLADEEP

**Session Classification:** (DCMMP) M2-4 Materials | Matériaux (DPMCM)

**Track Classification:** Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)