



Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: 4380 Type: **Oral Competition (Undergraduate Student) / Compétition orale (Étudiant(e) du 1er cycle)**

(UG*) Enhancing the Performance of Thermoelectric Materials by Integrating Computational Modelling and Machine Learning

Tuesday, May 28, 2024 3:15 PM (15 minutes)

This research aims to enhance the performance of thermoelectric systems through a multifaceted approach combining computational modeling and machine learning techniques. The study focuses on analyzing quantum statistics within thermoelectric systems to uncover novel insights into alloy doping. We verified key derivations concerning the extrema of thermal, lattice thermal, and electrical conductivities as a function of temperature. Utilizing the analytical equations proposed by Yadav et al. (2019), we numerically verified and validated these equations, and discussed the theoretical predictions given in the paper. We developed a machine-learning model to predict thermoelectric figures of merit. With the use of the Polylogarithm and Lambert W functions, the model aims to provide optimal values for doping in thermoelectric alloys and seeks to identify compositions that can significantly enhance thermoelectric performance. This study involves a comprehensive analysis of the interplay between doping concentration, material properties, and thermoelectric efficiency. Our study endeavours to provide valuable insights into materials that advance thermoelectric technology to develop more efficient and sustainable energy conversion systems.

Keyword-1

Thermoelectric Materials

Keyword-2

Machine Learning

Keyword-3

Mathematical Modelling

Primary authors: NAIR, Malavika (University of Western Ontario); LI, Xiyuan (University of Western Ontario); Prof. DESHMUKH, Pranawa (Indian Institute of Technology, Tirupati); Dr ROBERTS, Ken (University of Western Ontario); Dr JISRAWI, Najeh (University of Western Ontario); Prof. VALLURI, Sree (University of Western Ontario)

Presenter: NAIR, Malavika (University of Western Ontario)

Session Classification: (DCMMP) T2-7 Material Properties | Propriétés des matériaux (DPMCM)

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