Crystal Structure Prediction by Machine Learning

Date: Monday, March 22nd, 2021
Time: 11: 00 AM
Location: https://kfupm.zoom.us/j/94273755664

Speaker:
Fahhad Al-Harbi
Professor, Electrical Engineering Department
KFUPM

Abstract:

Data-driven material informatics have become an important part in materials science. Arguably, this could be the needed key to have considerable breakthroughs in accelerated materials discovery. In the past few decades, the existing materials data is enriched considerably by many computational materials initiatives. This naturally led to the adaptation of data analytics and machine learning to search for new materials. However, as common in computational sciences and applied mathematics, many incline toward applications while few focuses on the mathematical foundations and fundamentals development. This raises a serious concern of "black box" implementations which is unfortunately common. Furthermore, there are few general-purpose models to predict materials properties just from the chemical formula. Most of the ML applications so far are not general purpose and/or are applied merely to specific family of solid-state materials. In this talk, I will briefly present the team plan to develop "General Purpose Physically Guided Machine Learning Predictors of Materials Properties" and some recent developed efficient ML models to predict ionic radii, bond length, and crystal point groups.

Bio:

Fahhad H Alharbi obtained his PhD degree in electrical engineering with distinction from the University of Colorado at Boulder in 2004, and the MS. and BS. degrees from King Fahd University for Petroleum and Minerals (KFUPM) with high honors in 2001 and 1997 respectively. Before joining KFUPM as a faculty, he worked for Saudi Aramco, King Abdulaziz City for Science and Technology (KACST), IBM Inc., and Hamad Bin Khalifa University and its Qatar Energy and Environment Research Institute (QEERI). He is a professor in electrical engineering at KFUPM and his current research interest are in device physics (with emphasis on solar cells), the development and applications of new methods for large-scale atomistic calculations, machine learning for computational materials design, and multi-objective multi-scale materials inverse design.