Development of Machine Learning Potentials for Multicomponent Systems

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Chemistry Seminar on *The use of Machine Learning in Materials Chemistry*

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Abstract: Developing the interatomic potential models for muti-component systems has been "the holy grail" in the field of computational materials science. In this talk, I will discuss the use of Machine Learning as the means to address this issue quite effectively. With the advancement of GPU resources and GPU-based neural network algorithms, we have a great opportunity nowadays to utilize ML potentials to simulate a wide range of materials phenomena and processing in various scales. Typically, the potential development starts from the database generation through electronic structure calculations within the DFT approximation at ground state as well as elevated temperatures. The subsequently extracted critical data (of energy, stress, and forces) is then fed to the neural network with various schemes of invariant/equivariant representations. The key here is the linear scalability associated with these AI-driven models which in turn enable us to develop large scale atomic-based simulations with potential technological implications. Within this context, I would like to also discuss the feasibility in constructing AI-powered *Virtual* Autonomous Materials Discovery (*v*-AMD) to help accelerate materials development.

About the speaker: *Dr. Sakidja is a 2003 graduate of the University of Wisconsin Madison (UW-Madison) with a PhD in Metallurgy under the guidance of Prof. John H. Perepezko. After completing his school, he worked for the Department of Materials Science and Engineering at UW-Madison both as a lecturer and as a materials scientist with his mentors Prof. John Perepezko and Prof. Dane Morgan. In Spring 2013, he moved to the University of Missouri-Kansas City (UMKC) as an associate research professor in the Department of Physics & Astronomy collaborating with Curators' Distinguished Physics Prof. Wai-Yim Ching on the areas of electronic structure calculations, ab-initio molecular dynamics simulations and materials genome for high-temperature structural intermetallics and amorphous silica. In Fall 2014, he joined Missouri State University (MSU) as an associate professor in the Dept. of Physics, Astronomy and Materials Science (PAMS). In Fall 2019, he obtained his full professorship. He teaches physics and materials science core courses to undergraduate and/or graduate students including fundamental physics, computational physics, math methods, E&M, applied quantum mechanics, structure of solids, materials thermodynamics, scanning electron microscopy and computational materials science. His research interests span from developing high temperature and high-strength protective coatings, ceramics & alloys, designing nano-scale assemblies/layers to accelerating discovery and synthesis processes of functionalized hybrid structures. He serves as the director of Materials Science Graduate Program in the Dept. and is the recipient of an endowed Matthew & Patricia Harthcock CNAS Faculty Fellowship.*

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