SEMINAR NOTICE

Department of Physics and Engineering Physics
University of Saskatchewan

SPEAKER: Dr. Yansun Yao
Department of Physics & Engineering Physics

TOPIC: ***Machine Learning Accelerated Material Simulation***

DATE: November 2nd, 2021

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

PLACE:

ABSTRACT:

Join Zoom Meeting:
https://usask-ca.zoom.us/j/96818469630?pwd=aGpiVUtjcEJmZzBqclZ2S042eGpiQT09

Join by Telephone:
Local Saskatoon Dial-in Number: (639) 638-7474
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Join by Video Conferencing Device (SIP):
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Meeting ID: 968 1846 9630
Passcode: 07412447
Telephone Passcode: 07412447

I will introduce a new approach for simulating reconstructive phase transitions, which combines the Weighted Atomic Centred Symmetry Functions, Metadynamics Simulation and Machine Learning Representation of high-dimensional potential energy surface. The new method can reach the accuracy on par with the simulations based on Density Functional Theory (DFT), but with the computational cost several orders of magnitude less, and scaling with system size approximately linear. The accuracy of large-scale simulation is demonstrated by reproducing experimental phase transitions with unprecedented details, including nucleation, growth, and formation of different transition paths under particular stress conditions. With well-trained Machine Learning potentials, this method can be easily applied to all type of systems for accurate scalable simulations.