MATERIALS ENGINEERING

SEMINAR

"The Role of Local Atomic Environment Descriptors in the Effectiveness of Machine-learned Interatomic Potentials"

By

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ABSTRACT

In computational materials science, there is typically a trade off between the computational efficiency and the accuracy of calculations. This has traditionally been the case with density functional theory (DFT) and interatomic potentials (IAPs) where there is a choice between greater computational efficiency and accuracy. Recent work on describing the potential energy surface for structures with machine learning interatomic potentials (MLIAPs) has achieved accuracy approaching that of DFT while also maintaining longer temporal and length scales. This has been enabled by atomic structure descriptors with translation, rotation, and permutation invariance in conjunction with advanced modelling techniques such as neural networks. There is significant interest in using the most efficient set of structural descriptors as higher quality predictions can be made with greater computational ease. CUR decomposition is used to calculate the importance of features in order to compare two types of local atomic environment descriptors: bispectrum components and atom-centered symmetry functions (ACSF).

Date: Thursday, December 8, 2022
Time: 1:00pm
Place: PGSC (Grad Student Center on Northwestern), 105A
or WebEx via https://purdue.webex.com/join/strachan

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