Materials Science & Engineering Seminar Series

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Materials Science & Engineering

presents

Machine Learning for Alloy Modeling

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ABSTRACT:
We demonstrate the power of machine-learned potentials to model multicomponent systems. We compare two different approaches: Moment tensor potentials (MTP) and he Gaussian Approximation Potential (GAP) framework (kernel regression + the Smooth Overlap of Atomic Positions (SOAP) representation). Both types of potentials give excellent accuracy for a wide range of compositions and rival the accuracy of cluster expansion, even on benchmark systems. While both models are able to describe small deformations away from the lattice positions, SOAP-GAP excels at transferability as shown by sensible transformation paths between configurations, and MTP allows, due to its lower computational cost, the calculation of compositional phase diagrams. Given the fact that both methods perform as well as cluster expansion would but yield off-lattice models, we expect them to open new avenues in computational materials modeling for alloys. We show compositional phase diagrams, phonon dispersions, new superalloy phases, all predicted using these two machine-learned interatomic potentials for binary and ternary alloys.

BIOGRAPHY:
I study materials physics. I want to help change the world by inventing algorithms for discovering the materials of tomorrow, today. I am a professor in the **Department of Physics and Astronomy** at **Brigham Young University** (BYU). I also serve as an Associate Dean in the **College of Physical and Mathematical Sciences**. Before coming to BYU, I was an assistant professor at Northern Arizona University (NAU). Prior to my academic appointments, I worked in the Solid State Theory Group with Alex Zunger at the **National Renewable Energy Laboratory**. I received a Ph.D. from Univ. of California, Davis under Barry M. Klein.

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