**Title:** Phonon machine learning
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**Abstract:** Phonons are collective lattice vibrations in solids and play a key role various functional properties. However, phonon calculations have been experiencing high computational cost, while phonon measurements with momentum resolution have high technical barrier and limited resources. Beyond static properties, phonon transport with a mode-resolution has been challenging to acquire. In this seminar, we introduce three of our recent efforts aiming to acquiring phonon properties with the aid of machine learning.

First, we introduce the direct prediction of phonon density-of-states using atomic coordinates as input [1]. By using symmetry-aware graph neural networks to augment data, high-quality phonon density-of-states prediction is achieved with comparable performance with ab initio calculations but with much reduced computational cost. This enables a search for alloys for superior thermal transport.

Second, we introduce an integrated experiment-computational framework that can extract frequency-resolve phonon relaxation and transmittance based on ultrafast diffraction patterns. ultrafast diffraction offers high-dimensional data in time-momentum space where phonon thermal transport is reflected on the atomic vibrations and thereby diffraction intensities, and scientific machine learning is used to solve an inverse thermal transport problem and extract those frequency-resolved phonon transport with significantly increased reliability [2].

Finally, we introduce our latest work on predicting phonon spectra at Brillouin zone center and arbitrary k-points, by designing an alternative and generically applicable approach that can augment graph neural networks [3]. The method enables rapid and high-precision calculation of phonon bandstructure calculations in nearly arbitrarily complex materials, such as alloys, amorphous materials, or materials with very large unit cell with thousand atoms. A new phonon database containing phonon spectra of more than 100,000 materials are constructed.

[1] Zhangtao Chen et al., Direct prediction of phonon density of states with euclidean neural networks, *Adv. Sci.* 8, 2004214 (2021).
[2] Zhangtao Chen et al., Panoramic mapping of phonon transport from ultrafast electron diffraction and scientific machine learning, *Adv. Mater.* 2206997 (2022).
[3] To be posted online in Jan 2023.