Leverage Electron Properties to Predict Phonon Properties via Transfer Learning for Semiconductors

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Electron properties are usually much easier to obtain than phonon properties. The ability to leverage electron properties to help predict phonon properties can thus greatly benefit materials-by-design for applications like thermoelectrics and electronics. Here, we demonstrate the ability of using transfer learning (TL), where knowledge learned from training machine learning models on electronic bandgaps of 1,245 semiconductors is transferred to improve the models, trained using only 124 data, for predicting various phonon properties (phonon bandgap, group velocity and heat capacity). Compared to directly trained models, TL reduces the mean absolute errors of prediction by 65%, 14% and 54% respectively for the three phonon properties. The TL models are further validated using several semiconductors outside of the 1,245 database. Results also indicate that TL can leverage not-so-accurate proxy properties, as long as they encode composition-property relation, to improve models for target properties – a significant feature to materials informatics in general.