XenonPy.MDL: A comprehensive library of pre-trained models for materials properties

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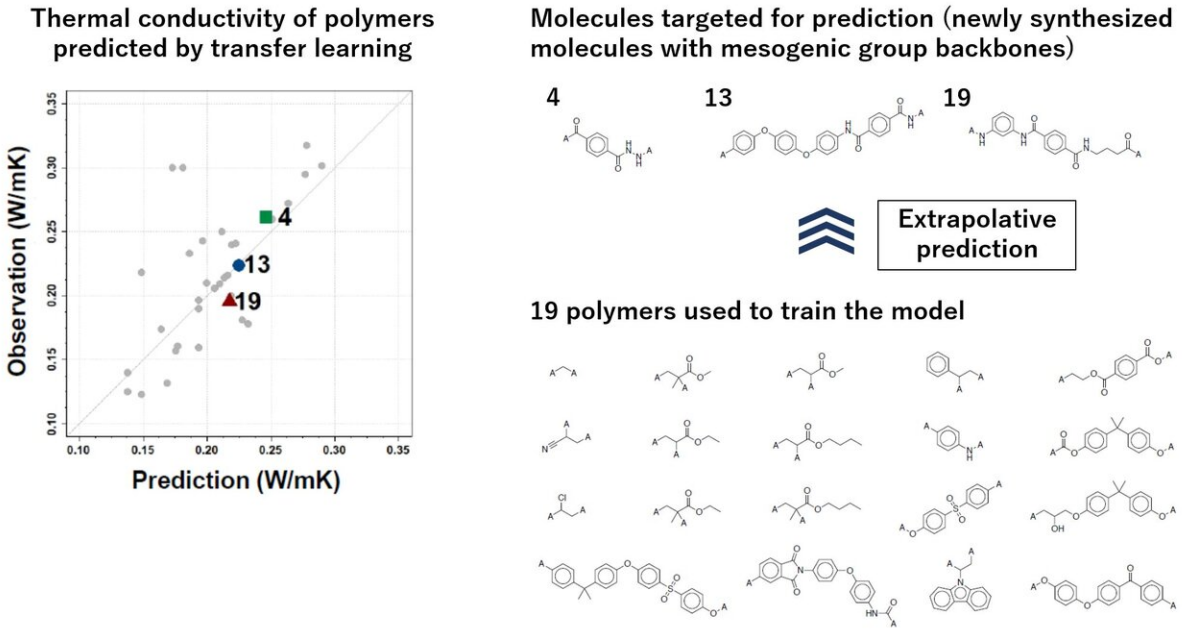

Thermophysical properties (i.e., thermal conductivity) of polymers predicted by transfer learning (TL). The joint research group succeeded in constructing a machine learning model capable of the extrapolative prediction of three new polymers that resided in far tails of the training data distribution (Yamada, Liu and others; ACS Central Science 2019). This was achieved by subjecting pre-trained models (e.g., models of the glass transition temperatures of polymers and of the specific heat capacities of small molecules) in the XenonPy.MDL library to transfer learning using only 19 sets of training data on the thermal conductivity of polymers. Credit: Ryo Yoshida

A joint research group consisting of the Institute of Statistical Mathematics (ISM) and the National Institute for Materials Science (NIMS) has developed approximately 140,000 machine learning models capable of predicting 45 different types of physical properties in small molecules, polymers and inorganic materials. The joint group then made XenonPy.MDL—a pre-trained model library—publicly available.

XenonPy—an open source platform for materials informatics (MI) research—was jointly developed by NIMS and a team at the ISM Data Science Center for Creative Design and Manufacturing. XenonPy uses machine learning algorithms to perform various tasks of MI. Users of XenonPy can run the pre-trained models available in the XenonPy.MDL library via the application programming interface (API) and use them to construct a variety of materials design workflows. The joint group recently reported the release of XenonPy.MDL in a research article published in *ACS Central Science*, a journal of the American Chemical Society.

In addition, as described in the article, the group succeeded in demonstrating the great potential of transfer learning to overcoming the problem of limited amounts of materials data in various MI tasks, for example, predicting the physical properties of small molecules, polymers and inorganic crystalline materials using exceedingly limited materials data.

More information: Hironao Yamada et al, Predicting Materials Properties with Little Data Using Shotgun Transfer Learning, *ACS Central Science* (2019). DOI: 10.1021/acscentsci.9b00804

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