

A General-Purpose Machine Learning Framework for Predicting Properties of Inorganic Materials

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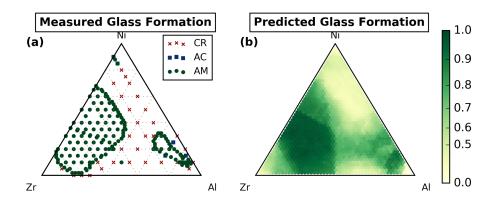


Figure.

Scientific Achievement

Machine learning models offer the ability to accurately predict the properties of materials much faster than conventional computational tools. However, one issue limiting their widespread use of these models is the lack of established procedures for creating them. In our new paper, we propose a general-purpose method for creating machine learning models from materials data. What is particularly exciting is that we found that this method can create accurate models for applications as different as crystalline solar cells and amorphous metal alloys without any problem-specific modifications.

Significance

This new method drastically simplifies the construction of machine learning models for materials properties, which will enable faster development of these useful models for many different materials engineering challenges.

Citation

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