Machine Learning–Accelerated Prediction of Amorphization Enthalpy in Ionic Compounds

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Amorphous materials have attracted significant attention due to their superior mechanical[1], electronic[2] and thermodynamic[3] properties compared to crystalline materials, positioning them as promising candidates for advanced applications in energy storage, electrocatalysis, and optical devices. Yet, systematic approaches to assess the amorphization propensity of various ionic compounds remain underdeveloped. Here, we present a data-driven framework to predict the amorphization enthalpy of ionic compounds (including oxides, nitrides, sulfides, and halides), providing a universal metric for the thermodynamic cost of transforming a crystalline phase into its amorphous counterpart. By integrating a standardized DFT-based melt-and-quench protocol with machine learning, we constructed a training set of 407 compounds and identified key descriptors influencing amorphization enthalpy. Although a random forest regressor highlighted relevant features, its predictive power was limited. To address this, we implemented e3nn[4]—a state-of-the-art graph neural network—and employed a transfer-learning approach. First, the model was pretrained on a larger dataset to predict shear modulus and subsequently fine-tuned on our amorphization enthalpy dataset. This strategy substantially improved prediction accuracy, allowing us to screen 12,123 ionic compounds from the Materials Project[5]. Our findings indicate that nitrides and sulfides generally resist amorphization, whereas alkali- or halogen-rich compositions promote it, and that multi-cation complexity can reduce the amorphization enthalpy. Overall, this framework provides a practical pathway for guiding experimental efforts in the discovery and fabrication of amorphous ionic materials for diverse applications.

Figures

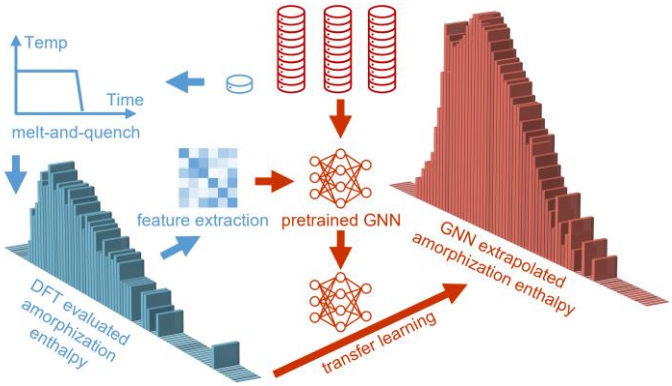

Figure 1. Schematic overview of data-driven framework for predicting amorphization enthalpy.

References

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