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Topology-Informed Machine Learning for Predicting Glass Stiffness

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Discovering novel glasses with enhanced properties and functionalities is essential to address many energy, communications, and infrastructure challenges. To this end, data-driven machine learning techniques offer a promising approach to accelerate glass discovery. However, although traditional machine learning models excel in interpolating existing datasets, they usually fail at extrapolating predictions far from the training set. This is a serious drawback since it limits their ability to identify new promising glasses in compositional domains that are yet to be explored—and such glasses are the most likely to feature properties that are very different from those of present glasses. Here, we present a new “topology-informed” machine learning framework that overcomes this limitation. We show that embedding some information about glass topology in machine learning models greatly enhances their ability to offer robust predictions far from their training sets.