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Abstract

Composition-property models based on machine learning (ML) have shown great promise in predicting oxide glass properties, but since they typically do not embed any physics knowledge, they struggle to predict properties outside of the compositional range used for training. There is therefore a need to inform ML models with knowledge of how glass composition affects short-range structure, but experimental structure data is not readily available for multicomponent glasses. To address this challenge, we here use statistical mechanics to inform a composition-structure ML model. This combined model offers an improved prediction of non-linear composition-structure relations in oxide glasses compared to models relying solely on statistical physics or machine learning individually. Importantly, the model is able to extrapolate predictions outside its training set, as it is able to predict the structure of a new glass series that was kept fully hidden from the model during its training.