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Designing the Network Former Speciation in Oxide Glasses using Statistical Mechanics

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Predicting the compositional evolution of the atomic-scale structure, particularly the network former speciation, in oxide glasses is important for tailoring their macroscopic properties. Experimental and computational techniques such as nuclear magnetic resonance (NMR) spectroscopy and molecular dynamics (MD) simulations, respectively, have successfully been used to understand the local structural environment of typical network formers such as silicon, phosphorous, and boron in simple glass systems. However, prediction of the structural speciation in multicomponent glasses with mixed network formers remains challenging. Here, building on the NMR and MD results, we present a statistical description of the compositional evolution of short-range structural units in multicomponent oxide glasses. This is done by accounting for the relative enthalpic and entropic contributions to the bonding preferences in binary former-modifier systems. These parameters are then transferred to predict the structural evolution in more complex multicomponent glasses without additional free parameters or input from any experimental data.