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Predicting Q-Speciation in Binary Silicate and Phosphate Glasses using Statistical Mechanics

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(GOMD-S1-023-2018) Predicting Q-Speciation in Binary Silicate and Phosphate Glasses using Statistical Mechanics

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Predicting the compositional evolution of the atomic-scale structure of oxide glasses is important for developing quantitative composition-property models. In binary silicate and phosphate glasses, addition of network modifiers generally lead to depolymerization of the networks as described by the Q-speciation. Upon the initial creation of non-bridging oxygens and thus partly depolymerized Q species, a variety of network former/modifier interactions exists. Here, based on ^{29}Si and ^{31}P magic angle spinning nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of Q-speciation in these glasses by accounting for the relative enthalpic and entropic contributions to the bonding preferences. We show that the entire glass structure evolution can be predicted based on experimental structural information for only a few glass compositions in each series. The model also captures the differences in bonding preferences in glasses with different field strengths of the modifier cations.