



## Statistical Mechanical Approach to Predict the Structure Evolution in Phosphate Glasses

Bødker, Mikkel Sandfeld; Mauro, John C.; Goyal, Sushmit; Youngman, Randall E.; Smedskjær, Morten Mattrup

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## Statistical Mechanical Approach to Predict the Structure Evolution in Phosphate Glasses

Mikkel S. Bødker<sup>1</sup>, John C. Mauro<sup>2</sup>, Sushmit Goyal<sup>3</sup>, Randall E. Youngman<sup>3</sup>, Morten M. Smedskjaer<sup>1</sup>

1. *Department of Chemistry and Bioscience, Aalborg University, Denmark*

2. *Department of Materials Science and Engineering, Pennsylvania State University, USA*

3. *Science and Technology Division, Corning Incorporated, USA*

Predicting the compositional evolution of the atomic-scale structure of oxide glasses is important for developing quantitative composition-property models. In binary phosphate glasses, addition of network modifiers generally lead to depolymerization of the networks as described by the Q-speciation, but involves a variety of different network former/modifier interactions. Here, based on <sup>31</sup>P magic angle spinning nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of Q-speciation in phosphate glasses with alkali, magnesium, and zinc modifiers by accounting for the relative enthalpic and entropic contributions to the bonding preferences.<sup>1</sup> 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. Finally, we also discuss the possibility to extend the statistical mechanical model to binary silicate and borate glasses.

<sup>1</sup> Bødker M. S., Mauro J. C., Goyal S., Youngman R. E., Smedskjaer M. M. Predicting Q-Speciation in Binary Phosphate Glasses using Statistical Mechanics. *J. Phys. Chem. B* **122**, 7609-7615 (2018).