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Modeling Oxygen Tricluster Formation in Calcium Aluminosilicate Supercooled Liquids and Glasses

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Abstract Body: Calcium aluminosilicate glasses have technological importance for a variety of industrial applications. However, the short-range structure of this glass system remains widely debated regarding the formation of oxygen triclusters. It is argued that triclusters are observed in high percentages within molecular dynamics simulations because of the high melting temperatures and correspondingly high fictive temperatures. This work explores the formation of such structural units by first simulating various compositions at different liquid temperatures to understand thermodynamic factors affecting the formation of such species. Structural results are then implemented into a statistical mechanical model which can predict the formation of triclusters at a given fictive temperature. Results show temperature and composition dependence of these structures, with aluminum charge modification favored in the peraluminous regime. It is concluded that oxygen triclusters are the preferred method of charge compensation even when extrapolating to laboratory fictive temperatures.