

A NMR-Driven Reverse Monte Carlo Study of Sodium Borate Glasses

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View Abstract

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CURRENT SESSION: Session 5: Atomistic Simulation and Predictive Modeling of Glasses

PRESENTATION TYPE: Contributed (Oral)

TITLE: A NMR-Driven Reverse Monte Carlo Study of Sodium Borate Glasses

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ABSTRACT BODY:

Abstract Body: Borate glasses are known to have a large fraction of the boron atoms involved in superstructural units like boroxol or pentaborate rings, in addition to the double coordination of boron atoms (3 and 4). This generates the boron's anomaly, which is a non-linear evolution of properties upon the addition of sodium oxide. In this work, we investigate theoretically and experimentally the structure of sodium borate glasses using ^{11}B and ^{23}Na NMR, classical and ab-initio molecular dynamics (MD) simulations and neutron diffraction.

We observe that only aiMD produces structural models with a non-negligible fraction of super-structural units (6 membered rings) but still below the one determined by two-dimensional ^{11}B MQMAS NMR. In order to improve our structural models, in particular to include a larger fraction of superstructural units, we develop a hybrid reverse monte carlo (HRMC) scheme combining MD with NMR and neutron data, taking the fraction of superstructural units as an adjustable parameter. Neutron data are found to be not sufficiently sensitive to

discriminate the various structural models, in contrast to ^{11}B NMR for both BO_3 and BO_4 units (i.e., ring and non-rings species). DFT computations of ^{11}B and ^{23}Na 2D MQMAS NMR are in good agreement with experiments.

KEYWORDS: Borate, NMR, Molecular Dynamics, Reverse Monte Carlo, DFT-NMR computations.

Presenter Acknowledgment: I have read and acknowledge the above paragraph

PROFESSIONAL/ACADEMIC STATUS:

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