Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Computational study on ionic diffusion and dynamic properties in silicate and bioactive glasses YE XIANG, JINCHENG DU, University of North Texas — Ionic diffusion and dynamic properties in silicate glasses have been extensively studied experimentally due to its importance in understanding ion conduction and glass dissolution. In this study, computational study on ionic diffusion and dynamic properties was carried out using molecular dynamics simulations with effective partial charge potentials. The simulated structure models were validated by comparing with experimental data and systematic discussions on effects of system size, simulation thermal ensemble and temperature range were carried out. The dynamic properties were also related to structural changes with the glass. Finally, investigation of SrO/CaO substitution effect on the diffusion behaviors in 45S glasses is provided.

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Date submitted: 03 Jan 2011 Electronic form version 1.4