

Molecular Simulation Studies of Water Speciation within Hydrous Silica Melts

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Molecular dynamics using Kohn-Sham density functional theory and Monte Carlo simulations using empirical potentials are used to examine the effects of water concentration in high temperature-high pressure silica melts. Understanding these melts is important for gaining insight into the chemical processes at work within the Earth's upper mantle. Of particular interest is the speciation of water within these liquids. Simulations performed over a range of state points ($2000 < T < 9000$ K, $0.25 < p < 10$ GPa, $0.0 < x(\text{water}) < 0.4$) show that water primarily dissociates and forms Si-O-H groups, even at high water concentrations (e.g., $x(\text{water}) = 0.4$). Gibbs ensemble Monte Carlo simulations are also used to explore the miscibility gap in these silica-water systems.