

First-principles simulations of structural and transport properties of silica liquid with/out water

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First principles molecular dynamics simulations show that water (8.25 wt%) has profound effects on the structural and transport properties of SiO₂ liquid over wide ranges of pressure (0 to 150 GPa) and temperature (3000 to 6000 K). We find that the melt structure changes substantially on compression. The speciation of the water component at low pressures is dominated by the isolated structures (with 99 % hydrogen participated) consisting of hydroxyls, water molecules, O-H-O bridging, and four-atom (O-H-O-H and H-O-H-O) groups. All hydroxyls are polyhedral (i.e. bound to Si atoms) whereas molecular water is mostly free. As pressure increases, these isolated structures increasingly combine with each other to form extended structures involving a total of five or more O and H atoms, which together consume over 75 % hydrogen at the highest compression studied. Water is shown to systematically depolymerizes the melt structure - the content of nonbridging oxygen (which is almost absent in anhydrous liquid) increased and the content of bridging oxygen decreased. Consistently, the dynamics of silica liquid is dramatically enhanced (higher diffusivities and lower viscosity) in the presence of water. At 3000 K, the diffusivities of all species (Si, O and H) and viscosity vary anomalously with pressure. The predicted dynamical changes are successfully associated with water-induced depolymerization of melt structure and water speciation, and the relevant microscopic mechanisms are revealed. Our predicted results here including those of MgSiO₃ liquid are expected to provide a fundamental basis for any dynamical model of magma ocean evolution.

Correlations of H₂O and S in the Martian midlatitudes

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Correlations between Mars Odyssey GRS-derived S and H₂O mass fractions in the planetary surface to several decimeter depths vary hemispherically, latitudinally, and across two regions of H₂O enrichment labelled 1 and 2 (Figure 1). Key observations include: (1) Areas of poor correlation (e.g. the Northern Hemisphere) contain extensive 'dust' mantles; (2) Circum-Arabia Terra (Region 1) shows the strongest correlation between H₂O and S; (3) H₂O and S may be weakly correlated even where H₂O is enriched, as in Region 2 roughly SE of Central Elysium Planitia and W of Medusae Fossae; and (4) even where H and S are strongly correlated and ice is unstable, much of the H may not be chemically bound in sulfates. Consistent with *in situ* observations at Meridiani and Gusev, the computed hydration state of potential divalent sulfates is in the 1 – 3 range at regional spatial scales.

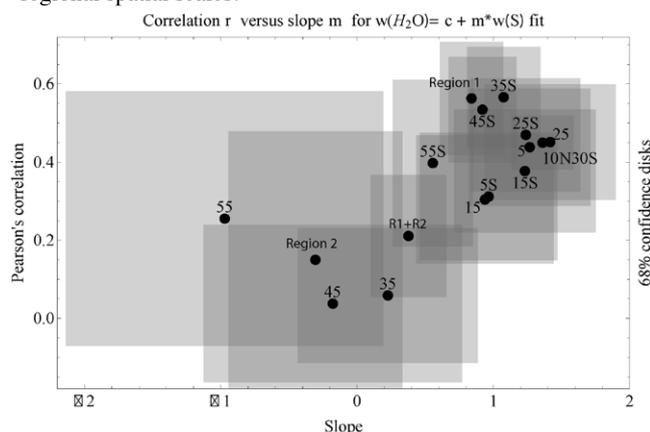


Figure 1: Prefix "S" denotes southern 10° - latitudinal bands, Regions 1 and 2 H-enriched regions, "R1+R2" Regions 1 and 2 combined, and "10N30S" 10° N to 30° S.

Characterization of surface properties within the two H₂O enriched regions with MRO-HiRISE imagery may help to reveal the underlying reasons for their contrasting H-S correlations. Analyses of H-Cl-S multivariate space may also clarify the potentially dominant role of non-sulfate hydrated minerals.