

**LETTER**

**The influence of atomic size and charge of dissolved species on the diffusivity and viscosity of silicate melts**

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**ABSTRACT**

Molecular dynamics simulations are used to determine how a dissolved species alters the transport properties of a silicate melt. To identify the specific factors that affect the transport properties, we examine the effects of generic dissolved species for which the atomic interaction parameters can be systematically varied. We focus on the role of the size and charge of the dissolved species. Our results show that neutral dissolved species have negligible effects on the structure and bonding of the silica network, regardless of the size of the species. These neutral species are decoupled from the network, and can diffuse orders of magnitude faster than the network ions. In contrast, charged species strongly disrupt the silica network, which leads to significant enhancement of the transport properties (e.g., lower viscosity and higher diffusivity of the network ions). The effects of the charged dissolved species are strongly dependent on their size.

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