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Viscosity of carbonate melts at high pressures and temperatures

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Knowledge about the viscosity and other transport properties of $CaCO_3$ melts at high pressures and temperatures relevant to the Earth's mantle is critically important for understanding the deep carbon cycle [1,2]. We have conducted First-Principles Molecular Dynamics Calculations of $CaCO_3$ melts up to 52.5 GPa and 3000 K to provide atomistic insights into the mechanisms of diffusion and viscosity. Our calculated viscosities of $CaCO_3$ melts at low pressures are in good agreement with those from experiments. In particular, viscosity is almost constant at low pressures but increases linearly with pressure above 10 GPa. The ultralow viscosity of $CaCO_3$ melts at low pressures [1] is readily attributed to the uncorrelated diffusion of Ca^{2+} and CO_3^{2-} ions (Fig. 1). In contrast, the motions of the Ca^{2+} cations and CO_3^{2-} anions at pressures >10 GPa become increasingly correlated (Fig. 1), leading to higher viscosities. Compared to water, the viscosity of $CaCO_3$ melts is not anomalously low. Rather, the viscosity of water is anomalously high, because water molecules are strongly H-bonded and behave like polymers.

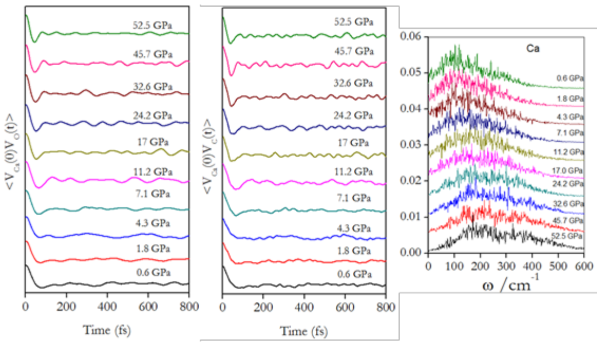

Figure 1: left and middle panels show the velocity cross correlation between Ca with O and Ca with C. Right panel is the vibrational DOS to highlight the emergence of a band at 400-500 cm^{-1}, showing the Ca-O vibrations.

[1] Kono et al. (2014) *Nature Commun*. **5**, 5091. [2] Wu et al. (2015) *Geophys. Res. Lett*. **42**, 5820-5827.