Dynamic ionization and superionic state of water under extreme conditions

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The behavior of water at extreme conditions of pressure and temperature is of profound importance to the planetary and geosciences, fundamental chemistry, environmental science, and biology. A superionic phase has been theoretically predicted above 20 GPa and at 2000 K [1], but has not been confirmed in more recent calculations [2]. Experimental studies include shock wave data to 26 GPa [3] and observations of the melting line up to 90 GPa [4-6], but no in situ characterization of water at extreme conditions is reported above 22 GPa.

Raman spectroscopy in a laser heated diamond anvil cell and first principles molecular dynamics (MD) simulations have been used to study water in the temperature range to 1500 K and at pressures to 56 GPa. We find a substantial decrease in intensity of the O-H stretch mode in the liquid phase with pressure and a change in slope of the melting line at 47 GPa and 1000 K. In agreement with these observations, theoretical calculations show that water beyond 50 GPa consists of very short lived (<10 fs) H_2O, H_3O^+ and O^{2-} species and that the mobility of the oxygen ions decreases abruptly with pressure, while hydrogen ions remain very mobile. We suggest that this regime corresponds to a superionic state, while water above the melting curve is dynamically ionized.

References:

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