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First-principles calculations of the high-pressure melt line of SiO2 and strength of H2O: planetary science implications AMIT SAMANTA, SEBASTIEN HAMEL, TINGTING QI, LLNL — We report the results from high-pressure high-temperature quantum molecular dynamics simulations of two materials of importance to planetary science. First, the high-pressure melt line of SiO2 using constrained free energy calculations under condition relevant to the Outer Planets. Second, we explore the stability of the H2O super-ionic phase by calculating the elastic constants at finite temperature and provides insight into the generation of magnetic fields of Uranus and Neptune.

Sebastien Hamel
LLNL

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