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Boiling of silicate liquids: a thermodynamic and molecular dynamic analysis

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Improved constraints on the thermodynamic properties of liquid-saturated silicate vapour would facilitate more accurate modelling of the planet and satellite-forming processes associated with giant impacts. We are developing a new equation of state (EoS) for fluids in the Si-O system in the hope of remedying mismatches between prediction and experiment associated with existing models. Our work has two components. (1) We reassess the available experimental information, and use it to parameterise a molecular equation of state (EoS). Unlike previous models, our model allows SiO_2 liquid to dissociate at high temperature, consistent with experimental observations. (2) Ab initio molecular dynamics simulations are underway to investigate the density of silica liquid at the relevant conditions of high temperature and low pressure.