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An Equation of State for Supercritical H_2

-Silicate Mixtures in Sub-Neptunes

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Many Sub-Neptune planets are thought to consist of molten "cores" (silicate mantle +/- discrete metal core) overlain by dense H_2-rich atmospheres. Sub-Neptunes likely contain significant masses of hydrogen in their interiors as the result of being built from planetary embryos that had their own H_2-rich atmospheres, in addition to ingassing. To investigate the nature of silicate-hydrogen interactions at temperatures and pressures relevant to these plants, we use density functional theory molecular dynamics (DFT-MD) simulations. Experiments and initial first-principles simulations suggest that $MgSiO_3$ and H_2 may show substantial miscibility at sub-Neptune conditions.

In this work, we use DFT-MD simulations to construct an equation of state (EOS) for supercritical $MgSiO_3$-H_2. We simulate silicate melt with dissolved hydrogen at high temperatures (4000–6000 K) and varying pressures, tracking density variations as a function of pressure. The pressure-density data are extracted from these simulations and fit using Birch-Murnaghan third and fourth order EOS models. Preliminary results indicate that hydrogen incorporation significantly lowers melt density. The densities are considerably lower than pure $MgSiO_3$ melt (e.g., 1.3 g/cc vs 2.6 g/cc at 5 GPa and 4000 K), and are similar to those obtained by mixing molar volumes of pure H_2 and $MgSiO_3$ at high P and T, although not identical.