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Immiscibility between hydrogen and molten iron in planetary interiors

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Hydrogen is a likely light element candidate in planetary cores. A hydrogen solubility limit in molten iron could determine the maximum amount of hydrogen possible in the core of a rocky planet. Here, we use ab initio molecular dynamics to investigate the liquid iron-hydrogen system at 10, 50, and 136 GPa and at high temperatures where iron is molten. We calculate Gibbs free energy of mixing at several compositions, from pure iron to hydrogen, using thermodynamic integration. We find that at 10 GPa and 3000 K, there is a liquid-liquid miscibility gap; iron and hydrogen unmix to form $Fe_{0.34}H_{0.66}$ and H_2. At 50 GPa, >2500 K and at 136 GPa, >3500 K, the melts are fully miscible. We extrapolate the Gibbs free energy of mixing to estimate the iron-hydrogen phase diagram down to 1 GPa and in the 1500-6000 K temperature range. As pressure increases, the liquid-liquid miscibility gap shrinks: the solubility limit of hydrogen in liquid iron increases and the closure temperature decreases. At 1 GPa, we estimate the solubility is 18 at% (0.38 wt%) hydrogen at 1500 K. The gap has completely closed by 38 GPa and 3000 K, 69 GPa and 2000 K, and 94 GPa and 1500 K. Thus, small bodies like moons, planetesimals, Mercury, and Mars, which have core-mantle boundary pressures under 30 GPa, are the most limited in the amount of hydrogen their cores can accommodate. On the other hand, iron and hydrogen are fully miscible at the core conditions of larger planets like Earth, Venus, super-Earths, and sub-Neptunes, so their hydrogen concentrations will be limited by sources during formation rather than a thermodynamic limit.