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Equation of State, Structure, and Transport Properties of Iron Hydride Melts at Planetary Interior Conditions

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Iron hydrides are a potentially dominant component of the liquid cores Earth and other differentiated rocky bodies, especially because of hydrogen's ubiquity in the universe. Using ab initio molecular dynamics, we examine iron hydrides with compositions up to 60 atomic% hydrogen at the high-pressure and -temperature conditions of planetary interiors. As hydrogen concentration increases, the melts are lubricated by hydrogen: iron and hydrogen generally become more diffusive, and the melt becomes more inviscid. Assessment of chemical speciation in the melts shows that there is minimal self-interaction between hydrogen at the conditions studied, i.e., it remains dissolved in iron. We parameterize a pressure-volume-temperature-hydrogen concentration equation of state. Our equation of state allows estimation of the physical properties of liquid iron cores within hydrogen-rich moons, exoplanets, and Solar System bodies.