

## 第一原理計算による地球外核条件下における液体鉄合金の研究 Liquid iron alloys with light elements at outer core conditions by first-principles calculation

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Since the density of the outer core deduced from seismic data is about 10% lower than that of pure iron at core pressures and temperatures (P-T), it is widely believed that the outer core includes one or more light elements. Although intensive experimental and theoretical studies have been performed so far, the light element in the core has not yet been identified. Comparison of the density and sound velocity of liquid iron alloys with observations, such as the PREM, is a promising way to determine the species and quantity of light alloying component(s) in the outer core. Here we report the results of a first-principles molecular dynamics study on liquid iron alloyed with different concentrations of light elements, in order to clarify the effects of their impurities on the liquid density and sound velocity under outer core P-T conditions. We also discuss validity of empirical Birch's law between density and sound velocity in liquid iron alloys.

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