Liquid Iron Alloys with Light Elements at Outer Core Conditions by First Principles

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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. Here we examine the density and bulk sound velocity of iron alloys with light elements, $(Fe,Ni)_x(H, Si, O, S, C)_{1-x}$, at Earth's outer core pressure and temperature conditions (~100 to 350 GPa, 4,000 to 7,000 K) based on first-principles molecular dynamics calculations. From molecular-dynamics results of binary alloys, density and bulk sound velocity of $(Fe,Ni)_x(H, Si, O, S, C)_{1-x}$ are estimated by ideal mixing. By comparing them with PREM, we constrain chemical compositions of the outer core which are compatible with PREM. Our results show that hydrogen and oxygen is a very potential candidate of light elements in the outer core, when the inner-core boundary temperature is relatively low and high, respectively. On the other hand, carbon is less preferable than other candidates. Based on the present results, we will be able to constrain light element composition further by taking into account other conditions: coexistence (e.g., Si and O cannot coexist in liquid iron alloys under the outer core condition), melting points, element partitioning between outer and inner cores, geochemical consideration, etc.

Keywords: Chemical composition of Outer core, Liquid iron alloys under high pressure, First principles

