He and Ar partitioning between liquid iron and molten silicate at high pressure

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The Earth’s core has been suggested as a potential reservoir of noble gases, which can remove the difficulties of their long-term maintenance in the mantle. The fundamental process controlling noble gas sequestering into the core is their partitioning between liquid iron and molten silicate. Unfortunately, limited measurements have only been conducted so far. Experiments conducted by Matsuda et al. [1993] up to 10 GPa showed that the partitioning coefficients of noble gases decrease with pressure, denying the core to be a noble gas reservoir. In contrast, Bouhifd et al. [2013] reported that the helium partitioning coefficient becomes more constant ($\sim 10^{-2}$) at $P > 10$ GPa, suggesting that some helium could be dissolved into the core. However, it is unclear whether this tendency is applicable to other noble gases.

Here we investigate the helium and argon partitioning between liquid iron and molten silicate using the ab initio molecular dynamics method combined with thermodynamics integration technique [Taniuchi and Tsuchiya, 2018]. The partitioning coefficients are computed from the Gibbs free energy changes associated with their exchange reactions. Although more detailed studies on several factors including temperature, pressure, and composition are required, our results in the moment suggest possible partitioning of helium and argon into liquid metal at high pressure. We will try to explain the behaviors from the electronic and structural points of view.

Keywords: Noble gas partitioning, Ab initio Calculation, Earth’s core