

Computational modelling of Iron isotope fractionation in solid and molten FeS metal alloys

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Iron is one of the most abundant non-volatile elements in the solar system and plays a major role in planetary formation and differentiation. Information about these processes can be gained by studying the Fe isotope fractionation. In particular, recent attention has been paid to $^{56}\text{Fe}/^{54}\text{Fe}$ equilibrium isotope fractionation at conditions relevant to Earth's core formation and the influence that light elements (O, H, C, Ni, Si and S) have had in this process [1]. Most of these experiments have relied on the study of Fe fractionation from quenched phases (silicate glasses and molten iron alloys). In addition, because of the difficulty of performing these experiments at high pressure, crystalline iron is often used as a proxy form of molten iron at deep conditions. In this work, we use ab-initio computational methods to perform a systematic study of the $^{56}\text{Fe}/^{54}\text{Fe}$ equilibrium isotope fractionation in molten and solid $\text{Fe}_x\text{S}_{(1-x)}$ alloys at conditions of the core formation. These data allow us to discuss the effects of using isotope fractionation data from solid metals as proxy for molten alloys at these conditions. Additionally, we comment on the effects of S concentration on Fe isotope fractionation in liquid systems. Finally, we discuss our findings on view of latest results on $^{56}\text{Fe}/^{54}\text{Fe}$ equilibrium isotope fractionation and their relevance for the formation of the Earth's core.

[1] Jin Liu *et al.* Nat. Comm. 8, 14377 (2017)