Iron isotope migration between silicate mantle and metallic core

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Iron has participated in all early planetary processes including accretion and core-mantle segregation and in turn, those events might have left imprints on Fe isotopic composition. Thus far, the fractionation of Fe isotope has been greatly employed to understanding the formation and evolution of terrestrial planets[1,2]. Here we show that iron forms chemical bonds of strong strengths in pyrite-type FeO_2Hx at high pressures[3-5], about twice that in iron alloys. From the measured mean force constants of iron bonds, we calculate an equilibrium iron isotope fractionation of about +0.1 ‰ between pyrite-type FeO_2Hx and iron under the Earth's core-mantle boundary conditions, which is comparable to the shift of terrestrial basalts. Our result shows that pyrite-type FeO_2Hx forming in the core-mantle boundary region would be enriched in heavy Fe isotopes. This study suggests that FeO_2Hx may be an effective source of heavy iron isotopes for ocean island basalts if it is raised upwards by mantle plumes to the shallow part of the mantle.

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3 Hu, Q. *et al.* FeO2 and FeOOH under deep lower-mantle conditions and Earth's oxygen–hydrogen cycles. **534**, 241 (2016).
4 Liu, J. *et al.* Hydrogen-bearing iron peroxide and the origin of ultralow-velocity zones. *Nature* **551**, 494-497 doi:10.1038/nature24461 (2017).
5 Liu, J. *et al.* Altered chemistry of oxygen and iron under deep Earth conditions. *Nat. Commun.* **10**, 153, doi:10.1038/s41467-018-08071-3 (2019).

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