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Ab initio and machine learning-based simulations of hydrogen in the Earth's core

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The physical and chemical state of Earth's core is challenging to match using only pure iron. An additional amount of light element(s) is required to account for its geophysical features (e.g., core density deficit), and among various candidates proposed in the Earth's core [1], hydrogen attracts special attention: (i) It is the most abundant element in the universe and, due to pressure stabilization of iron hydrides FeHx (where x denotes nonstoichiometric H), substantial hydrogen might have been sequestered into the core during planetary accretion. (ii) FeHx reproduces not only the density and compressional velocity of the outer core, but also the anomalously high Poisson's ratio of the inner core [2]. (iii) Low solidus temperatures of pyrolite at core–mantle boundary pressure conditions require a substantial reduction of the melting temperature of the outer core by impurities [3]; hydrogen is known to depress the melting temperature of iron more efficiently than other alloying elements. Given that a substantial amount of hydrogen likely is present during planetary differentiation, whether, and to what extent, hydrogen was stripped from the bulk silicate Earth into the core hinge primarily on the hydrogen partitioning behavior between metallic and silicate melts. In this talk, I will present our recent efforts to constrain the hydrogen partition coefficients between silicate and iron, and between liquid and solid iron determined by (i) Gibbs energy calculations using Kohn-Sham (KS) density functional theory (DFT)-based thermodynamic integration methods, and (ii) large-scale two-phase coexisting simulations. In the latter approach, to bypass the computational cost of solving the KS equations while representing potential energy surfaces at KS-DFT accuracy, we build a neural network potential that directly uses relative atomic coordinates to describe local atomic environments to obtain atomic energies and forces. With these simulation results, I will discuss the hydrogen compositions of the bulk, inner and outer core.

[1] K. Hirose, B. Wood, and L. Vočadlo, Nat. Rev. Earth Environ. 2, 645 (2021).
[2] W. Wang, Y. Li, J. P. Brodholt, L. Vočadlo, M. J. Walter, and Z. Wu, Earth Planet. Sci. Lett. 568, 117014 (2021).
[3] R. Nomura, K. Hirose, K. Uesugi, Y. Ohishi, A. Tsuchiyama, A. Miyake, and Y. Ueno, Science 343, 522 (2014).

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