

Partitioning of hydrogen at Earth's inner core boundary: Implications for compositions of the Earth's core

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Recent studies indicate that the Earth's core can be a reservoir of hydrogen¹⁻³, so the substantial amounts of hydrogen in the core may be essential to constraint the composition of the Earth's core. The outer and inner core compositions are interconnected because the inner core crystallized from the outer core⁴. Unlike sulfur, silicon, oxygen, and carbon, hydrogen is accommodated at interstitial sites in metal. A fast method is developed to calculate the chemical potential of hydrogen in Fe-H alloys based on ab initio molecular dynamics in conjunction with the neural network and the test particle method. We observe that the partition coefficient of hydrogen between the outer core and the inner core is 0.29~0.43 under 6200 K and 330 GPa. Hydrogen cannot be the only light element in the Earth core based on the partition coefficient and density limit. With seismological observations and geochemical constraints (partition coefficients of other light elements), we estimate the compositions of the outer core (Fe+5.0% Ni+0.069~0.34% S+ 4.1~5.7% Si+ 4×10^{-3} ~0.12% O+ 2.9×10^{-3} ~0.023% C+ 0.37~0.48% H by weight) and the inner core (Fe+5.0% Ni+0.052~0.26% S+ 4.1~5.7% Si + 0.11~0.15% H by weight).

References

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