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Ab initio calculations of iodine core–mantle partitioning: Implications for heterogeneous accretion

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Mid-ocean-ridge basalts (MORBs) and ocean island basalts (OIBs) display distinct xenon isotope patterns, revealing processes dating back to Earth's early accretion[1,2]. Specifically, OIBs display a lower $^{129}Xe^*_{I}/^{136}Xe^*_{Pu}$ ratio compared to MORBs[3-6], likely due to heterogeneous accretion and potentially influenced by core formation, as experiments indicate that iodine becomes increasingly siderophile under higher pressures[7-10]. However, understanding iodine partitioning between the core and mantle is complicated by the effects of sulfur and oxygen content in the core, hindering accurate quantification of accretion processes. Here, we performed ab initio thermodynamic calculations to determine iodine partitioning between silicate melt and liquid iron alloys with varying S and O contents. Although we find that iodine becomes more siderophile with increasing S and O contents in liquid iron, it remains lithophile and largely partitioned to the mantle within the core's maximum S and O levels. Therefore, core formation could not significantly deplete iodine from the bulk silicate Earth, attributing the xenon isotope disparity between MORB and OIB sources to heterogeneous accretion. Using I-Pu-Xe isotope systematics, we constrain the late veneer contribution to between ~0.07% and 1.68% of CI material or its equivalent in other carbonaceous chondrites.

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