Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11581

How do I and Pu partition during core formation? Constraints from first-principles molecular dynamics and implications.

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In silicate portions of our planet, part of ^{129}Xe comes from the beta decay of now extinct ^{129}I (^{129}Xe*) and part of ^{136}Xe comes from fission of extinct ^{244}Pu (^{136}Xe*$_{Pu}$) and extant ^{238}U. High-precision data on ocean-island basalt samples (thought to originate from deep mantle plume) revealed a uniformly low ^{129}Xe*/^{136}Xe*$_{Pu}$ ratio in the lower mantle compared to mid-ocean-ridge basalt (MORB) samples (originating from upper mantle) [1]. This difference in ^{129}Xe*/^{136}Xe*$_{Pu}$ ratio has been attributed to deep and shallow mantle reservoirs having different initial I/Pu ratios, which would be established during Earth's accretion. Specifically, two models have been proposed: (i) a heterogeneous volatile accretion history for the Earth [1], or (ii) partitioning of iodine into liquid metal during core formation [2]. Identifying which of these hypotheses is correct is critical to our understanding of Earth's evolution. Indeed, in the first case, highly volatile elements (including iodine) would be depleted in early accreted material compared to later building blocks of the Earth, which would be inefficiently mixed into the proto-Earth's mantle. In the second scenario, a change in the nature of Earth's building blocks is not required. However, the geochemical behaviour of plutonium at high P and T conditions, relevant to core formation, remains unexplored.

Here, we apply first-principles molecular dynamics simulations [3] to calculate the partition coefficients of I and Pu between liquid iron and silicate melt at high pressures and temperatures. We find that Pu, which is lithophile at ambient mantle conditions, becomes siderophile at higher temperatures. Using multistage core formation models exploring different plausible accretion scenarios, we find that I and Pu are unlikely to be sufficiently fractionated to explain the plume/MORB difference during homogeneous volatile accretion. Instead, our results are consistent with a protracted phase of accretion of volatile depleted materials, followed by a final accretion phase of volatile-rich materials, as proposed by [1]. We will discuss the most likely nature of these materials, and the implications for Earth's accretion history.

[1] Mukhopadhyay (2012) Nature 486, 101-104. [2] Jackson et al. (2018) Nature 553, 491-495. [3] Zhang & Yin (2012) PNAS 109, 19579-19583.