Ab initio prediction of potassium partitioning into the Earth's core

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Silicate earth is in strong depletion of K compared with chondrites [Wasserburg, 1964, Science]. The ratios of K isotope barely vary suggesting evaporation cannot be responsible for the missing of K [Humayun and Clayton, 1995, GCA]. The finding that the change in electronic structure of K from alkaline- to transition metal-like at high pressure highlighted the possibility of its incorporation into the core [Parker, 1996, Science]. If K is present, even in ~ppm, the radiogenic heat produced by ^{40}K could be an important energy source for mantle dynamics [Labrosse, 2001, EPSL]. However, previous researches didn't enclose the controversy over the K partitioning behavior between silicate and metallic system, with its partitioning coefficient range from 10^{-6} to 2.5 [Bouhifd etal., 2007, PEPI; Watanabe, 2014, PEPI], leaving the K content in the core uncertain.
In this study, ab-initio molecular dynamics simulations are performed to investigate whether and how much K can enter the metallic system. K partition coefficients are determined by Gibbs free energy changes of its exchange reactions between silicate and metallic systems. Helmholtz free energy is obtained based on "thermodynamic integration" by computing the difference between two systems with different potential energy functions.
Our preliminary results show that the K content entered into the core is limited, though it would be affected by the temperature, pressure, composition of the metallic (the type and content of light elements) and silicate system (NBO/T).

Keywords: Ab-initio simulation, Potassium, Core Mantle Boundary

