Light Elements in the Core and Their Constraints on the Timing of the Moon-forming Giant Impact

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The degree of chemical equilibration (hereafter as *Ke*), defined as the cumulative mass fraction of the metalic core in equilibrium with the silicate mantle during the Earth accretion processes, greatly influences determination of the timing of the Earth core formation [1]. If *Ke* is larger than ~0.4, Hf-W chronology implies a fast accretion in less than 30 Myr for the Earth. Otherwise, Hf-W data can only be used to constrain the Ke instead of timing [1]. Here we use the two-phase first-principles molecular dynamics (FPMD) [2] to constrain the solubility of light elements in liquid iron in equilibration with silicate melt at temperatures from 2500 to 4200 K, pressures from 20 to 120 GPa, and two compositions simplified from the "O-bearing" and "Si-bearing" bulk Earth model compositions of McDonough [3]. The solubility data are then used in the simulations of the many possible accretion scenarios of the Earth as outlined in [4], considering magma ocean depth, homogeneous vs heterogeneous accretion etc. For each accretion route, we calculate the effective core-mantle equilibration degree (*Ke*),

$$K_e = \sum_i^N Ke_i \times W_i$$

where Ke_i and W_i are the core-mantle equilibration degree and the accreted mass fraction of the ith step, respectively. The successful *Ke* are selected based on the criterion that the resulting Earth's core must meet the required density deficit [5]. The *Ke* in those successful simulations are all found to be larger than 0.57, implying that the core-mantle differentiation has to occur early [1], within 30 millions years from the beginning of the solar system as originally stated [6]. We show [7] that FPMD calculations lend strong support to the classical geochemical mass balance approach in accessing light elements in the core [3].

[1] Rudge *et al* (2010) *Nature Geosci* **3**, 439. [2] Zhang & Guo (2009) *GRL* **36**, L18305. [3] McDonough (2003) *Treatise Geochem* **2**, 547. [4] Rubie *et al* (2011) *EPSL* **2**, 301. [5] Birch (1952) *JGR*, **57**, 227. [6] Yin *et al* (2002) *Nature* **418**, 949. [7] Zhang and Yin (2012) *PNAS* **109,** 19579