

# Mass Transport and Structural Properties of Liquid Iron Alloys at high pressure from *ab-initio* simulations

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Earth's core is composed mostly of an Fe-Ni alloy with substantial yet unknown concentrations of additional elements. The question of core composition is particularly important because it directly relates to the conditions under which the core formed during accretion. It is well known from a comparison of seismic observations and shock wave or static experiments that the Earth's core must contain significant amounts of elements lighter than iron. The onset and evolution of Earth's geodynamo is also intimately related to the core's light alloy budget due to their chemical buoyancy associated with fractional crystallization of the inner core. Geophysically significant elements alloying with Fe and Ni in Earth's core must satisfy a number of requirements: (i) high cosmochemical abundance, (ii) solubility in liquid iron under conditions of the core-mantle differentiation, and (iii) matching density and sound wave velocities of the bulk alloy liquid with seismic observations. The geophysically most interesting and discussed alloy components for the Earth's core are H, C, N, O, Mg, S, Si, and Ni. The incorporation of alloying elements in solid metals is well understood to be controlled by the radius ratio of a central and packing atoms. Although liquids fundamentally lack long-range periodicity, their short-range order can be used to make realistic predictions of "liquid packing structure" which in turn can be used to estimate the dominant incorporation mechanism (i.e., substitutional or quasi-interstitial) of a given alloying element. Importantly, when the compressibilities of two atom types differ significantly, coordination values will vary as a function of  $P$  and  $T$ , which can affect solubility and partition coefficients. The compression behavior of liquid iron alloys over a planetary-scale  $P$ - $T$  range is therefore particularly relevant for estimating alloying element behavior under conditions beyond those accessible in the laboratory. We determine mass transport and structural properties of binary liquid iron alloys over a wide density (5.055-11.735 g/cm<sup>3</sup>) and  $T$ -range (2,500–6,500 K) using first-principles molecular dynamics. Compositions consist of 96 at% Fe and 4 at% light element (H, C, N, O, Mg, Si, S, or Ni). Self-diffusion coefficients ( $D$ ) of Fe and the alloying elements range from  $3.5 \cdot 10^{-9}$  to  $1.9 \cdot 10^{-7}$  m<sup>2</sup>/s, and results show a relation between mean atomic radius and  $D$  ratios for the alloying element and iron: Si and Ni are "iron-like" with similar atomic radii and  $D$  compared with those of Fe; H, C, N, O, and S are "small non-iron-like" with smaller atomic radii and larger  $D$ ; Mg transitions from "large non-iron-like" with a larger atomic radius and smaller  $D$  at low density to iron-like under conditions of the Earth's core. The effect of pressure on  $D$  for C, N, and O is negligible for densities below  $\sim 8$  g/cm<sup>3</sup>, accompanied by an increase in average coordination numbers to  $\sim 6$ , and an increase in mean atomic radii. For densities above  $\sim 8$  g/cm<sup>3</sup>,  $D$  and atomic radii of these elements decrease monotonically with  $P$ , which is typical for the iron-like alloying elements as well as for H, Mg, and S over the whole compression range. While atomic radius ratios move toward unity with compression, diffusivity ratios for the alloying element relative to iron tend to increase for the "non-iron-like" elements with density.

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