

Stable carbon isotope fractionation in the Fe-C system from first principles

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Carbon is the fourth most abundant element in the solar system and likely one of the constituent light elements in the Earth's core. Determination of its equilibrium isotope fractionation factor (α) under high pressure (P) and temperature (T) is a key for understanding chemical evolution such as the whole Earth carbon distribution and the amount in the Earth's core. It is still unclear how carbon isotope fraction creates the isotopic variation in the deep Earth formed during the core-mantle segregation. Recently, we have initiated the theoretical determination of the α in the Fe-C system in the Earth's deep interior with a full *ab initio* approach based on the density-functional theory. We performed *ab initio* lattice dynamics calculations for diamond and iron-carbide (hexagonal (h) Fe₇C) having the two stable carbon isotopes (¹²C and ¹³C). The α between the two phases were then determined by using the Gibbs free energies calculated under the whole lower mantle P,T conditions. The heavier carbon is found to be more enriched in the diamond than in iron carbide, which is consistent with that observed in the low- P experimental study (Satish-Kumar et al., 2011). Our calculations show that the $\delta^{13}\text{C}$ values of diamond and h-Fe₇C₃ are about $\sim -20\%$ (0-100 GPa and 2000-4000K). The values are close to that observed in carbonaceous chondrites, but it deviates from a widely accepted value of the bulk-silicate-earth ($\sim -5\%$). This indicates that the core-mantle interaction in an early stage may not have produced the observed distributions in the deep Earth.