Stable carbon isotope fractionation in 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 distributions and the amount in the Earth's core (e.g., Kumar et al., 2011). Because experimental measurement of the isotope fractionation remains technically challenging at the deep mantle condition, attempts to evaluate the α among mantle minerals by first-principles calculations have been made in recent years (e.g., Huang et al., 2014). Recently, our group 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 Fe7C3) 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 at P ˜300 GPa and T ˜2000-6000 K. The obtained 103lnα dia-Fe7C3 is found to vary with T from ˜+8‰ (2000 K) to ˜+5‰ (6000 K). This result indicates that the Fe7C3 is enriched in the heavier isotope (13C) compared with diamond. This trend is qualitatively consistent with low-pressure experimental observations (Kumar et al., 2011).

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