

## **Constraints on iron isotopic fractionation from DFT calculations and NRIXS spectroscopy**

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Iron is a ubiquitous element, naturally abundant in all terrestrial reservoirs, starting from the Earth core made of metallic iron alloyed with some lighter elements. In order to investigate the complex geochemical behavior of iron in rocks, fluids and magmas, isotopes are essential tools and equilibrium fractionation factors represent reference data that are crucial for interpreting the measurements made on natural samples. These isotopic equilibrium constants can be derived from isotopic exchange experiments, but also from first-principles calculations (atomistic modeling based on quantum mechanics, mostly on density functional theory, DFT) and vibrational spectroscopies such as Mössbauer spectroscopy and nuclear resonant inelastic X-ray scattering (NRIXS). Confronting data obtained from these techniques enables to provide reliable equilibrium fractionation factors and in the meantime, improves our understanding of the parameters controlling the relative enrichment in heavy isotopes of the different phases. After reviewing available data for iron isotopes, we will talk about these controlling parameters, with as central parameter the interatomic force constant. Finally we will tackle more specifically the question of the equilibrium isotopic fractionation between liquid and solid phases. Due to technical limitations, silicate glasses are used as proxies for melts in NRIXS measurements. This approach will be discussed in light of recent DFT calculations made on liquid and solid phases of pure and alloyed iron metal.