

## **Theoretical investigation of Zn isotope fractionation**

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Understanding the biogeochemical cycle of zinc is of a great importance due to the economical, environmental and health implications. Indeed, half of extracted Zn from ore deposits is discarded to soils, which are the largest reservoir of this element after Earth's mantle and crust and Zn is an essential nutrient to living beings which can suffer from both its deficit and excess. Investigating the isotopic compositions is an efficient way to trace the sources and processes involving this element. The mobility of Zn is controlled by its interactions with the organic and inorganic constituents of soils. Processes like mineral precipitation, complexation in aqueous solution, adsorption on mineral surfaces, incorporation in secondary minerals, potentially induce a fractionation of Zn isotopes. The present study aims at determining the equilibrium mass-dependent isotopic fractionations associated with some of these processes. These key fractionation factors that may be difficult to obtain from controlled experiments in laboratory, obeys the laws of statistical and quantum mechanics. We thus obtain the equilibrium fractionation factors by performing first-principles calculations based on the density functional theory (static calculations, molecular dynamics and metadynamics).

We will present first the results for Zn-bearing minerals, covering a large variety of Zn crystallographic environments (Ducher et al. 2016). We will discuss the crystal-chemical properties at the origin of isotopic fractionations (interatomic bond strength, in turn controlled by bond lengths and atomic charges). We will briefly mention the issues related with the modeling of the hexaaquo zinc complex, before discussing the equilibrium isotopic fractionations between aqueous Zn and minerals. The calculated data set provides a consistent basis to interpret isotopic variations measured in the environment.

### **Reference**

Ducher M. et al. (2016) Chem. Geol., 443, 87-96