

## Theoretical equilibrium iron isotope fractionation factors between silicate minerals in the context of magmatic differentiation

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Understanding the processes involved in iron isotopes fractionation during magmatic differentiation is essential in order to use iron isotopes as tracers for planetary bodies formation. Over years, the systematic iron isotope fractionation in natural lavas has been interpreted as being driven by different processes such as: fractional crystallization, fluid exsolution, thermal diffusion, effect of oxygen fugacity or sulfide saturation (e.g. [1][2]). However, the significance of each processes are still debated because of the lack of a strong set of iron equilibrium fractionation factors between silicate minerals. In order to expand the dataset, first-principles calculations based on the density functional theory have been performed on olivines (Hortonolite, Fayalite), clinopyroxenes (Augite, Diopside, Hedenbergite, Aegerine), an orthopyroxene (Enstatite) and an oxide (Ulvospinel) that are the main Fe-bearing minerals in lavas. Comparisons with existing NRIXS measurements [3] and separate minerals analysis [4] will be presented. We will also discuss the crystal chemical properties at the origin of isotopic fractionations such as interatomic bond strength (charge and bond length) and the impact of the second atomic neighbour on iron.

### References

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