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Prediction of stable isotopes fractionation by first-principles methods.

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Quantitative modeling of isotope fractionation is a key-problem in geochemistry. Difficulties to extract information from empirical data, and to measure fractionation factors at low temperature for kinetic reasons, support the quest for alternative approaches to this problem. First-principles density functional theory has proved to be successful in reproducing the physical and chemical properties of many systems (Baroni et al. 2001). It is nowadays commonly used in fields such as molecular spectroscopy or mineral physics. Within this framework, we have recently developed a methodology which makes it possible to predict fractionation factors between solids as a function of temperature (Meheut et al. 2007). We will present recent theoretical results on the isotopic fractionation factors related to hydrogen, oxygen and silicon in the system quartz-kaolinite-water. Comparison with experimental data will make it possible to assess the precision of our approach (typically a relative error of 5 %) and will provide independant constrains on still poorly known fractionation factors such as the oxygen internal fractionation between OH and non-OH sites in kaolinite and the silicon fractionation (30Si/28Si) between quartz and kaolinite. Theoretical fractionation factors are 12 permil and 1.6 permil at 300K, respectively.

Bibliography

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