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First-principles modeling of stable isotope fractionation processes

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The analysis of the mechanisms controlling the stable isotope composition of natural compounds and the use of these isotopic compositions to elucidate natural processes is a central field of geochemistry. An essential basis for interpreting isotopic compositions is to know the equilibrium isotopic fractionation factors. These reference fractionation factors can be calculated using a statistical thermodynamic approach based on the vibrational properties (i.e. first-principles calculations based on the density functional theory). These theoretical tools enable us to link isotopic properties to speciation and crystal-chemistry, and therefore to investigate the molecular mechanisms controlling isotopic fractionations. The computational approach thus complements perfectly the experimental work performed under controlled conditions in order to fully apprehend natural environments through stable isotopes. This talk will show how first-principles calculations can contribute to isotopic geochemistry with recent examples focusing on the fractionation of non-traditional stable isotopes (Zn, Fe,...) for minerals and aqueous species in low-temperature conditions.