

## Prediction of B, Li and Si equilibrium isotope fractionation between minerals, aqueous solutions, melts and metals at high P and T

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“Non-traditional” stable isotopes of light elements such as B, Li and Si are important geochemical tracers widely used in petrology. B and Li isotopes strongly fractionate between minerals and fluids during fluid-rock interaction. The fractionation of Si isotopes between silicate melt and iron-rich metal during Earth's core formation is assumed to produce the observed difference in isotopic signatures between the Bulk Silicate Earth and Chondrite meteorites. In order to understand the origin of these isotopic signatures we need to know the equilibrium isotope fractionation factors between the different materials of interest. They can be determined in high P/T experiments, which due to extreme conditions is often a difficult task, or computed. In order to deliver the required information we have developed an efficient *ab initio* based computational method for prediction of the equilibrium isotope fractionation factors between different phases at high P and T, including fluids and melts. We have tested our method by computing the B and Li isotope fractionation factors between complex B/Li-bearing crystalline solids (tourmaline, staurolite, spodumene and micas) and aqueous solution, and by comparison of the results with the existing experimental data. We show that we are able to reproduce correctly the experimental isotope fractionation sequences: fluid-tourmaline-mica for B and staurolite-fluid-mica-spodumene for Li and compute the fractionation factors with an uncertainty comparable to the experimental error [1]. In addition, we are able to get a valuable atomic-scale insight into the processes driving the fractionation of isotopes, such as coordination environment of cations, or speciation in fluids [1,2]. The computations also provide a better understanding of the experimental results such as “contradicting” measurements of B isotopes fractionation between mica and tourmaline [2]. With our method well tested on B/Li systems we attempt to derive the fractionation factors of Si isotopes between silicate melt and iron-rich metal fluid at the condition of Earth's core formation. We believe that the results of such theoretical investigation will help to better constrain the Si fractionation factors and address the question on the silicon content of the Earth's core.

[1] Kowalski, P. M. and Jahn, S. (2011) *Geochim. Cosmochim. Acta* **75**, 6112-6123.

[2] Kowalski, P. M. Wunder, B. and Jahn, S. (2012) *Geochim. Cosmochim. Acta* submitted.

## Cd mobilization from Fe(III)-hydroxides by an isolated Fe(III)-reducing *Geobacter* strain and its impact on enhanced phytoremediation

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Habitats worldwide have strongly been contaminated with industrial waste metals, such as Cd, which may potentially enter the food chain through plants. These contaminant metals have drastic effects on human and environmental health. Hence, there is a demand for the development and application of new techniques to efficiently remediate contaminated soils.

In the present study, we present a new Fe(III)-reducing *Geobacter* strain, isolated from a highly Cd-contaminated soil in Germany. This *Geobacter* strain reduces Cd-loaded Fe(III) hydroxide fast and to a large extent and thus mobilizes the Fe-mineral-bound Cd. Using X-ray diffraction we identified and characterized the Fe(III) minerals present during and after Fe(III) reduction. Synchrotron-based STXM-XRF analysis was used to locate Cd in the cell-mineral aggregates. Taking into account the data presented in this study, Fe(III)-reducing bacteria could potentially mobilize Cd in Cd-contaminated soils and make it more bioavailable. We are currently investigating whether the mobilized Cd is taken up and accumulated by the Cd hyperaccumulator plant *Arabidopsis halleri*, leading to the net removal of Cd from the contaminated site. Hence, combining enhanced natural attenuation and phytoremediation could potentially be a technique to remove metals from contaminated sites more time- and cost-efficiently. First studies in plant-microbe-soil microcosms showed that the presence of the naturally occurring microbial community compared to sterile conditions leads to a higher uptake of Cd into the plant *A. halleri*, potentially due to the presence and higher activity of Fe(III)-reducing bacteria.