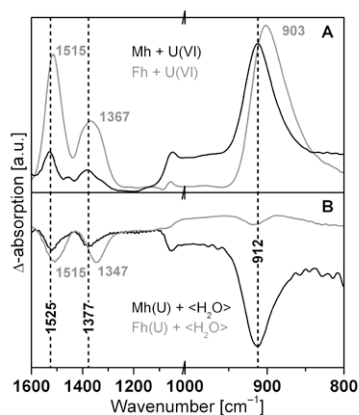


## Sorption and desorption processes of U(VI) on iron (hydr)oxide phases

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In this comparative study, the surface speciation of uranium(VI) on ferrihydrite (Fh) and maghemite (Mh) were investigated by vibrational spectroscopy. The experimental setup allows the monitoring of the surface processes at the water-solid interface in real time with a time resolution in the subminute time range. The performance of the experiments under inert gas atmosphere and under ambient conditions provides further insight into the molecular events of the binary and ternary sorption systems, respectively.



**Figure 1:** IR spectra of the sorption (A) and desorption (B) processes of U(VI) on ferrihydrite (Fh) and maghemite (Mh) in ambient atmosphere.

The spectra clearly demonstrate a characteristic surface speciation in dependence of the solid phase. On Fh, the formation of ternary inner sphere complexes are observed as it was derived earlier [1]. In addition, the time-resolved spectra reveal the change of the surface speciation of atmospherically derived carbonate upon U(VI) sorption [2].

From the sorption experiments on Mh, outer sphere complexation of the uranyl ion can be derived. In ambient atmosphere, contributions of carbonate ions to the U(VI) surface speciation on Mh can not be ruled out.

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## Physical properties of CO<sub>2</sub>-rich melts at mantle conditions: A simulation study

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There are growing evidences that CO<sub>2</sub>-rich melts play a key role in the geodynamics, chemical differentiation and degassing of the upper mantle. Experiments at HT-HP on carbonate-silicate assemblages suggest that the onset of mantle melting may start as deep as 300 km in generating carbonatitic melts at very low melt fraction [1]. The electrical conductivity anomalies measured in the asthenosphere by magnetotelluric sounding can be explained by the presence of highly conductive phases which could be CO<sub>2</sub>-rich [2,3]. On the other hand, the composition of primary magmas at the origin of hypabyssal kimberlites has been recently reevaluated and should be transitional between carbonate and silicate melt with low SiO<sub>2</sub> contents [4]. Furthermore it appears that the role and abundance of the carbonatite volcanism has been underestimated [5], and recent database and world distribution map of carbonatites [6] show that a carbonatitic magmatism was abundant from the late Archean to the Phanerozoic.

However, the physical properties of carbonatites and carbonated silicate melts are poorly known. Here we present an evaluation of the physical properties of CO<sub>2</sub>-rich melts by molecular dynamics (MD) simulation. This atomistic approach relies on the development of a realistic force field to describe the incorporation of CO<sub>2</sub> in a silicate melt [7] and that of a silicate component in a carbonate melt, as well. With this force field it has been possible to simulate a large composition range from carbonatites to CO<sub>2</sub>-saturated basalts with a special emphasis on the transitional compositions (0-15wt% SiO<sub>2</sub>). The EOS, the viscosity and the electrical conductivity of the simulated melts have been evaluated at mantle conditions. It is found that the composition has a large influence on the melt properties, a result which has important geophysical implications.

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