Carbon flow from volcanic CO_2 into soil microbial communities of a wetland mofette

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We investigated mofettes, i.e., cold Volcanic CO_2 exhausts, in a wetland area in the NW Czech Republic. Here, continous emanations of CO_2 lead to lower pH and anoxic conditions. Recent findings suggest that such alteration might cause a shift of the microbial community towards anaerobic and acidophilic organisms.

In this study we i) analyzed differences in the active archaeal and bacterial community structure in different depths of a mofette compared to the surrounding wetland soil by 16S rRNA pyrosequencing and ii) used DNA- and lipid-based ^{13}C-CO_2 Stable Isotope Probing (SIP) to identfy microbial communities which can incorporate the emanating CO_2.

16S rRNA pyrosequencing revealed that the overall active bacterial community composition was similar for the mofette and reference soil in all sampled depths. However, in the mofette soil *Acidobacteria* showed a higher relative contribution (55% to 70%) compared to the wetland reference (17% to 22%) primarily consisting of sequences closely related to Cand. *Koribacter* sp. and isolate „Ellin 624“ of Subdivision 1. The active archaeal community of the mofette soil was dominated by methanogens in all depths which were not represented in the wetland reference soil.

Analysis of incorporation of ^{13}C-labeled CO_2 into PLFAs and ether-lipid derived hydrocarbons in the mofette soil showed continuous enrichment over 28 days in almost all bacterial and archaeal biomarkers. Archaeal CO_2 utilization was restricted to the first 10 cm of the soil, while a depth-independent labeling pattern was found for bacterial biomarkers. Archaeal 16S rRNA and formyl tetrahydrofolate synthetase (*fhs*) gene labeling analysis of the first 10 cm suggested that $^{13}CO_2$ was potentially utilized chemolithoautotrophically by two novel groups of acetogens and methanogens, with the latter primarily being affiliated with the family *Methanoregulaceae*. On the other hand, bacterial 16S rRNA gene labeling analysis indicated a non-obligate autotrophic utilization of $^{13}CO_2$ by bacterial families of the *Anaerolineaceae*, unclassified *Bacteroidetes* and *Syntrophaceae*.

Characterization of hydrocarbon and functionalized silica nanoparticle adsorption on mineral surfaces through advanced First Principles techniques

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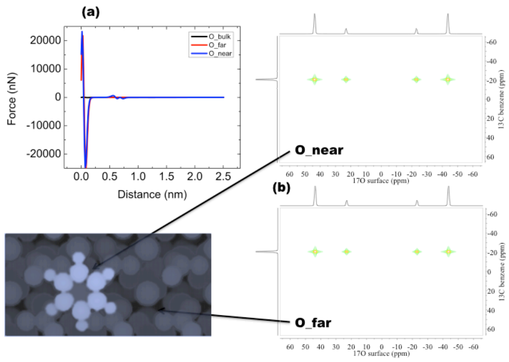
Atomistic simulations have come to play an increasingly important role in advancing understanding of the fundamental properties related to the hydrocarbon and nanoparticles interaction with mineral surfaces. In this work, we will present an integrated methodology based on First Principles methods to characterize the surface properties (structural, energetic and electronic) and the adsorption of hydrocarbons and funcionalized (hydroxylated, sulphonic acid and pegylated) SiO_2 nanoparticles within mineral surfaces (Carbonate and Silicates). The simulations were based on the Density Functional Theory (DFT) with solid state Nuclear Magnetic Resonance calculations (1) and simulation of noncontact Atomic Force Microscopy (nc-AFM) (2) including van der Waals corrections (3). It was possible to assign the peaks in the NMR spectra for all structures studied and determine the force distance models based on simulated AFM. Our results show a chemical shift differentiation for atoms located on different sites (bulk and surface) for calcite and silicate systems as well as the differences on force versus distance curves. Interestingly, the presence of hydrocarbon molecules also modifies the chemical shift of adsorbed the Ca and Si sites with respect to the pristine and isolated surfaces. Calculated AFM forces allow us the differentiation between the different chemical sites and a clear understanding of the adsorption processes. Within the combining theoretical AFM and NMR simulations with DFT with van de Waals, it should be possible to elucidate the coordination environment of chemical species in many important complex materials in the context of geochemical phenomena.



AFM forces(a) and (b) 2D ^{17}O-^{13}C spectra for benzene adsorbed on CaCO3 surface

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