Interaction of ions at the surface of soil components

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Complex structure of soil makes it interesting for both experimental and theoretical studies. One of most important components of soil, which has strong effect and play important role in the process of adsorption of different elements to the plants and complex formation process of many metal ions in the environment is natural organic matter (NOM).

Solvation structure and dynamics of building blocks of NOMs in aqueous solution studied and surface propensity to the air/aqueous interface observed and decrease of surface tension measured[1] which is supported by surface sensitive (VSFG) spectroscopy[2].

Also we have used the Temple-Northeastern- Birmingham (TNB)[3] model of humic acid which was proposed by Sein *et al*. for complex formation with different ions such as carbonate and iodate ions. We have observed that strong interactions between carboxylate groups of model humic acid take place both in protonated and not protonated hucmic acids. Moreover, hydrogen bonding and complex formation are two main factors which influencing the aggregation of model humic acid in aqueous solutions. Moreover, we studied the surface propensity and interaction of TNB with different organic contaminants such pesticides by classical molecular dynamics (MD) simulations and revealed that the hydrophbic interaction between organic contaminants and hydrophobic parts of humic acid is one of the most important factor for interactions and surface propensity to the air/aqueous solution interface.

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Textural control over electron transfer and reaction with Li^+ of biomineralized Fe-oxides

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The capacity of biominerals, in particular Fe-bearing minerals, to conduct electrons is increasingly studied with the aim of understanding the mechanisms by which bacteria can retrieve electrons from minerals [1,2] and designing electricity providing [3] or energy-storing devices [4]. Here, we present a two-step biomineralization pathway using the anaerobic Fe-oxidizing bacteria *Acidovorax sp*. strain BoFeN1 leading to the formation of α-Fe_2O_3 that was used in Li-ion batteries. Biomineralization of γ-FeOOH within the 40-nm thick cell wall of the bacteria [5], followed by a short heat treatment provided an alveolar material consisting of hollow rod-type shells made of an assemblage of nanometric and oriented α-Fe_2O_3 particles (Fig. 1A, B). This material exhibited enhanced electrochemical properties compared to abiotic controls, which relies on its specific texture at the μm- and nm-scales allowing increased electronic transfer and sustained reaction with Li^+ ions. These results have implications for energy storage and for understanding the mechanisms of electron/ion transfer through biominerals.

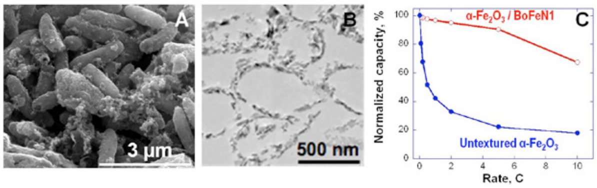

Figure 1: Texture of α-Fe_2O_3 bacteriomorphs biomineralized by BoFeN1 observed by SEM (A) and TEM in thin section (B). Electrochemical capacity-power (vs. Li^0) for textured and untextured materials (C).

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