[MS24-P10] Effect of Fe^{2+} and Fe^{3+} on amino acid adsorption on surfaces of iron oxide

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Magnetite (Fe_3O_4) crystallises in the inverse spinel structure [1]. In nature magnetite is also an important biomineral. Magnetotactic bacterias, e.g., use magnetite single-crystals to orientate themselves in the earth magnetic field. The connection between the inorganic magnetite and the organic parts of the animals is the magnetosome membrane (MM). This membrane is built by membrane proteins which are dominated by the amino acids aspartic acid (asp), glutamic acid (glu), glycine (gly) and leucine (leu) [2,3]. Bürger et. al [4] showed that it is energetically favourable for the amino acids to adsorb on the relaxed magnetite-(111)-surface. For the current study, the hematite-(001)-, the wuestite-(111)- and the unrelaxed magnetite-(111)-surface have been used. They are the most common surfaces of the respective minerals. Their crystal structures contain iron as Fe3+, Fe2+ and a mixture of both, respectively. However, in all systems studied the surface oxygen termination is the densed packed oxygen layer.

Force field simulations of the interaction between iron oxide surfaces and the amino acids offer the possibility to investigate if and how the amino acids interact with the surfaces. Additionally, it is possible to investigate the interactions and the adsorption distances between the surface atoms and the functional groups of the amino acids. We have chosen the COMPASS force field because all parameters of the surfaces and of the amino acids are defined in this force field. As simulation software we used Forcite which is integrated in the Materials Studio 5.0 software package.The amino acids may adsorb in a docking box of 43.9 Å x 43.9 Å x 20 Å on the wüstite-(111)-surface, in a docking box of 50.4 Å x 50.4 Å x 20 Å on the hematite-(001)-surface and in a docking box of 47.9 Å x 47.5 Å x 20 Å on the magnetite-(111)-surface. The surface thicknesses are 9.3 Å, 16.2 Å and 17.6 Å, respectively. For every amino acid-iron oxide system 10,000 frames has been calculated, resulting in 120,000 frames altogether. The lowest energy systems for each combination have been evaluated.

The comparison of these systems shows the resulting differences in the adsorptions behaviour.The adsorption mode switches between monodentate, bidentate and bridging obviously by the amount and oxydation state of the iron cations. The Fe-O adsorption distances between the surface Fe-atoms and the amino acids O-atoms vary between the twelve different adsorption systems, but in all different cases the electrostatic interaction dominates the process. The conformations of all of the four amino acids varies for the three different iron oxide surfaces.

In our study we show that the effects of the iron oxidation states takes distinct influence on the adsorption distance, the binding mode and especially the conformation of the amino acids.

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