Establishment of euxinic oceanic conditions following the Lomagundi Event

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Following the great oxidation event (GOE), the isotope record of marine carbonate rocks suggests a massive burial of organic carbon in an event known as Lomagundi excursion (LE). It is estimated that during this period atmospheric oxygen attained levels much higher than during GOE [1]. It is proposed that as the LE declined, oxygen dropped to lower levels [1, 2], but the direct geochemical evidence for the state of atmospheric and ocean oxygenation both during and after the LE is missing. This time window is also represented by the 2.2-2.0 Ga Francevillian group of Gabon, well known for the earliest large colonial organisms [3]. In order to investigate the nature of marine water-column chemistry, samples representing the entire section were subjected to multielement (C, S, Fe, Mo, U) biogeochemical study.

Geochemical data show deep water oxic conditions during deposition of the lower part of the section in agreement with the LE. Nevertheless the interlayered Mn deposits occured in ferruginous anoxic conditions reflecting sea-level changes. The upper part of the section reflect euxinic conditions, and together with δ^{98}Mo values, these data confirm a significant decrease in the oxygenation of ocean water in the aftermath of the Lomagundi Event.

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Hydration, structure and mobility of Cs^+ and Sr^{2+} in montmorillonite and muscovite clay minerals

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Clay minerals used as natural and engeenered barriers in geological nuclear waste repositories are able to considerably reduce the mobility of radionuclides in the environment. The radionuclide retention happens through a combination of various physical and chemical processes taking place at the clay-water interface, but their molecular mechanisms are still insufficiently understood.

To obtain detailed microscopic scale information on the structure, dynamics, and energetics of Cs^+ and Sr^{2+} ions at the surfaces of model illite and smectite clays (muscovite and montmorillonite, respectively) we have performed a series of classical molecular dynamics (MD) computer simulations using the CLAYFF force field [1]. New sets of structural models with different degrees of compositional disorder in the octahedral and tetrahedral layers of clay were constructed and investigated in order to quantify the effects of such disorder on the properties of the adsorbed ions.

The structural properties were probed in terms of the atomic density distributions in the direction normal to the clay surfaces, along the planes parallel to the clay surfaces, atom-atom pair correlation functions, and coordination numbers. The 2-dimensional and 3-dimensional diffusion coefficients were calculated to probe the ionic mobility at the clay surfaces and in the interlayer space. In the case of montmorillonite (a swelling clay), the hydration energetics was also systematically investigated by determining the hydration and immersion energies [2].

The atomic density profiles vary with the charge and size of the ions and show a significant layering at the interfacial regions of both studied clays. Pair correlation functions and coordination numbers indicate only one stable adsorption site for cations on the basal surface of muscovite (ditrigonal) in contrast to two adsorption sites on a similar montmorillonite surface (ditrigonal and triangular). Cs^+ and Sr^{2+} mobility is considerably reduced by substrate adsorption, but the diffusion coefficients tend to get closer to bulk solution values when the ions are removed from the surface.

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DOI:10.1180/minmag.2013.077.5.14