REE geochemistry of iron-apatite deposits in Central Iran

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REEs in different ore types display characteristic patterns, related to different modes of formation of the ore. The apatites of iron- apatite ores of Bafq region (Central Iran) show a strong LREE/HREE ratio and a pronounced negative Eu anomaly. This pattern is a distinct characteristic of igneous apatites. Mentioned REE pattern is similar to that of apatites from Kiruna iron ore and the other Kiruna- type iron ores in elsewhere of the world.

In the all Iron-Apatite deposits of Central Iran, the REE patterns of apatites, phosphate- bearing iron ores and iron ores with no or very little phosphate, are similar and have a different REE contents. This similarity indicates a common source for these rocks and deposits. On the other hand, the REE patterns of granitic intrusions which are located adjacent to the iron-apatite ores have a similar REE patterns to that of iron- apatite ores. This similarity, in turn, also indicates a genetic relation for these rocks.

In general, it can be consider a basic alkaline magma rich in iron and some incompatible elements such as P, REE, Th-U, Cl and F, have been parent magma for Iron-Apatite ores and granitic intrusions. This parent magma had been differentiated into immiscible silicate- oxide- phosphate units in route of ascend to the earth's surface.

# Modelling of nanoparticles: Aggregation of oxides and hydroxides

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We use molecular dynamics simulations to study the aggregation of CeO_2 (ceria) and $Mg(OH)_2$ (brucite) nanoparticles (NPs). Calculations are running in vacuum and in water in order to include the effect the solvent during aggregation. We employ the DL_POLY code [1] and a potential model fitted in the METADISE [2] and the GULP [3] codes against *ab initio* data derived using the VASP code [4]. We use ceria, an extended solid oxide, and brucite, a layered material, as models. Forcing oriented aggregation during the crystal growth of such important materials for catalysis and sorption processes can facilitate the production of tailor-made structures with enhanced properties.

The free energy change due to aggregation NPs can be evaluated considering different interparticle orientations. Results for 1ns run for ceria NPs in vacuum are shown in Figure 1. The calculations predict no free energy barrier to aggregation when the NPs approach along crystallographic orientations as previously reported by Spagnoli *et al*. [5]. Finally, a comparison between aggregation in dry and wet conditions is considered.
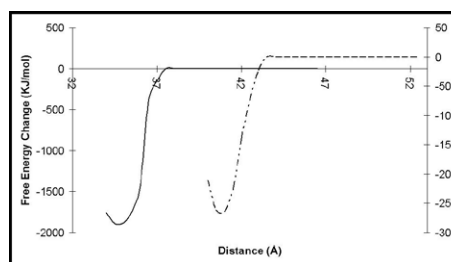
Figure 1: Free energy change of aggregation as a function of distance for a 5nm diameter octahedral CeO_2 NPs with a fixed orientations: dashed line, approaching edges; solid line, approaching faces.

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