Arsenic incorporation in FeS_2 Pyrite

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Iron-bearing sulfide minerals play an important role in the generation of acid rock drainage (ARD) and subsequent release of toxic elements such as arsenic. FeS_2 pyrite, the most abundant of all metal sulfides, can incorporate large amounts of arsenic (up to ~10 wt%), and thus its breakdown can pose a potential threat to the environment. Despite its importance, the location and speciation of arsenic in pyrite remains a matter of debate.

We are using Density Functional Theory (DFT) to calculate the energy of different arsenic configurations both on the surface and within the bulk pyrite lattice. Solution energies are determined by considering incorporation resctions under both oxidising and reducing conditions. Results suggest that arsenic will preferentially be incorporated in sulphur sites, forming As-S dianion groups. Substitution energies indicate that arsenic impurities will cluster, even for the low concentrations (<4 wt%) modelled here. Our results also show that, in oxidising conditions, the presence of arsenic may accelerate the dissolution of pyrite and hence the release of of toxic metals and generation of acid waters.