

# Unveiling the chemical reactivity of sulfide mineral surfaces in the presence of water and oxygen.

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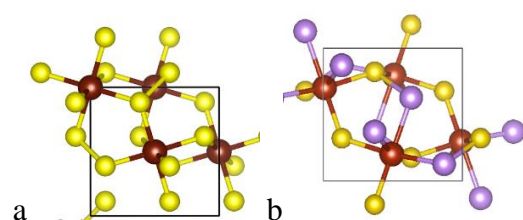
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Modeling chemical reactions that occur in the solid/water interfaces is challenging. A realistic model of the solid/water interface must include aspects such as surface reconstruction, defects in the solid, water dissociation, pH and ionic strength.

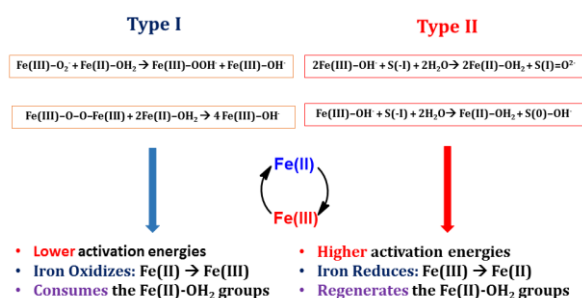
We have successfully modelled the oxidation mechanism of pyrite, FeS<sub>2</sub>, (Fig 1a) in the presence of water and oxygen using Density Functional/Plane Waves calculations<sup>1</sup>. Pyrite oxidation is an important environmental issue related to the mining of noble metals such as gold, copper and uranium. The oxidation of sulfide minerals leads to the formation of sulfuric acid contributing to the acidification of aquifers and, hence, the remobilization of heavy metals to the environment. We have shown that the adsorbed water on the surface has an important role participating in the oxidation process through an intricate sequence of reactions that can be summarized as shown in the Fig. 2. The experimental results are now adequately understood in terms of our proposed oxidation mechanism.

The arsenopyrite, FeAsS (Fig. 1b) is normally found associated to pyrite. The presence of the arsenic replacing one of the sulfur atoms have been subject of debate. It is shown that the presence of the As in the pyrite structure, will avoid some of the necessary steps to oxidize the arsenopyrite favoring its oxidation<sup>2</sup>. Furthermore, the pyrite/arsenopyrite interface form a galvanic pair that promotes the oxidation of the arsenopyrite with respect to the pyrite<sup>3</sup>. The stability and the band offset of the pyrite/arsenopyrite interface explains why the pyrite favors the oxidation of the arsenopyrite.

The sulfur oxidation due to the reconstruction of the chalcopyrite (CuFeS<sub>2</sub>) surface<sup>4</sup> with the formation of sulfide dimer and the formation of two dimensional crystal covellite (CuS) will be also discussed<sup>5</sup>.



**Figure 1.** Structure of a) pyrite and b) arsenopyrite. Sulfur in yellow, arsenic in blue and iron in red.



**Figure 2.** The types of reactions that occur on the pyrite surface in the presence of water.

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## References

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