

Theoretical investigation of chalcopyrite surfaces

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Sulphide minerals are involved in the extraction of many metals of economic importance and also with some phenomena observed in degraded areas such as acid mine drainage¹. The oxidation and leaching mechanism of the sulphide minerals is still a matter of debate. Chalcopyrite is an important sulphide mineral which is the main source of copper. Its composition is CuFeS_2 and its electronic structure is not completely understood.

The hydrometallurgical extraction of copper ores often involves the leaching of chalcopyrite. This process has received much attention due to the increasing need to treat chalcopyrite ores by hydrometallurgical processes. In the present work, we focused our investigation on the (001), (100), (110), (101), (111) and (112) surfaces aiming to understand the first step of the leaching mechanism. Density Functional Theory (DFT) calculations have been performed using the Quantum-ESPRESSO package – PWscf. Generalized gradient approximation (GGA) for the exchange and correlation potential (XC) due to Perdew and Wang (PW91) has been used. The electron-ion interactions are described through ultrasoft pseudopotentials. The results show strong reconstruction of the surface upon relaxation leading to the sulphur oligomers (S_n^{2-} , $n=2,3$) followed by the reduction of Fe(III) to Fe(II) center. These findings are in agreement with the experimental XPS results². Löwdin population analyses, density of states and electron localization functions have been used to understand the electronic structure of the chalcopyrite surfaces. Implications on the chalcopyrite surface reactivity will be discussed. In figure 1, the electron localization function for the reconstructed of the (001) sulfur terminated surface is shown.

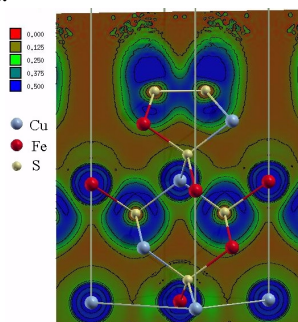


Figure 1. Electron localization function of the S-terminated surface. The lone electron pairs are shown.

[1] C. Klauber, *Int. J. Miner. Process* **86**, 1 (2008).

[2] S. L. Harmer, J. E. Thomas, D. Fornasiero, A. R. Gerson, *Geochim. Cosmochim. Acta* **70**, 4392 (2006).

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