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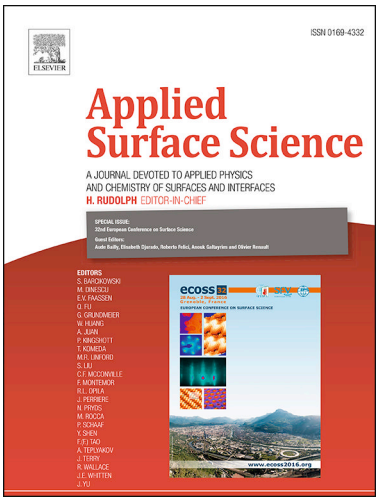

Full Length Article

Density functional theory study of cyanide adsorption on the sphalerite (110) surface

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Density functional theory study of cyanide adsorption on the sphalerite (110) surface

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Abstract: Cyanidation tailings in gold plants often contain lots of sphalerites that are difficult to recycle by flotation because of the strongly depressive effect of the residual cyanide. To reveal the depression mechanism of cyanide on sphalerite, the adsorption of isolated cyanide molecule (CN) at different coverages on the sphalerite (110) surface were studied by means of density functional theory. The calculated results show that the adsorption energy of per CN molecule drops as the increase of adsorbed CN molecule coverage, indicating that the adsorption structure becomes more thermodynamically stable. Cyanide molecule adsorption on sphalrite (110) surface prior occurs on the atop site of surface Zn atom, in which the Zn 3d orbital donates electrons to the 2p orbital of C forming a d-p back donating bond, leading to the production of hydrophilic zinc cyanide complexes that serve as strong obstacles to the flotation recovery of sphalerite in cyanidation tailings. Electron transfer from mineral surface to the adsorbed CN molecules takes place during the process of CN adsorption, and the surface atoms lose more electrons when the coverage of adsorbed CN molecules is high, weakening the reactive activity of Zn and S atoms on the sphalerite (110) surface.

Key words: Sphalerite; Cyanidation tailings; Surface adsorption; Density functional theory

1. Introduction

With high leaching rate and relatively low cost, cyanidation is the primary process for the extraction of precious metals in gold and silver mines nowadays, especially when the successful application of carbon-in-pulp technology is achieved [1-2].

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