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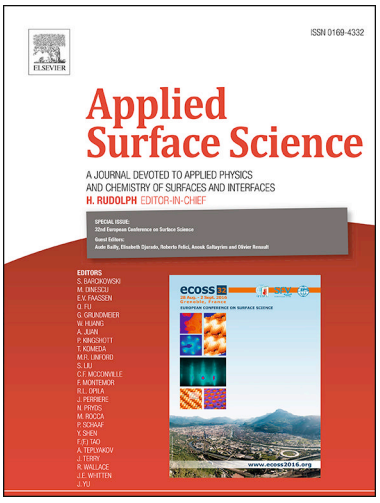

Full Length Article

DFT study of SDD and BX adsorption on sphalerite (110) surface in the absence and presence of water molecules

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DFT study of SDD and BX adsorption on sphalerite (110) surface in the absence and presence of water molecules

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Abstract

The adsorption of sodium dimethyl dithiocarbamate (SDD) and butyl xanthate (BX) on sphalerite (110) surface in the absence and presence of water molecules was simulated using density functional theory (DFT). The results indicated that both the SDD and BX can chemically adsorb on the sphalerite surface in the absence of water molecules. However, the presence of water molecules on sphalerite surface significantly increases the adsorption energy of SDD and BX, which is detrimental to SDD and BX attachment on sphalerite surface. Particularly, the presence of water molecules changes the adsorption of BX on sphalerite surface from chemisorption to physical absorption, but the adsorption of SDD on sphalerite surface is still very strong like that of chemisorption. The results of DOS comparison analysis, electron density and Mulliken population analysis also confirmed the adsorption of SDD on sphalerite surface is more easy and stable than that of BX adsorption.

Key words: Sphalerite; Dimethyl dithiocarbamate; Butyl xanthate; Surface adsorption; DFT

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