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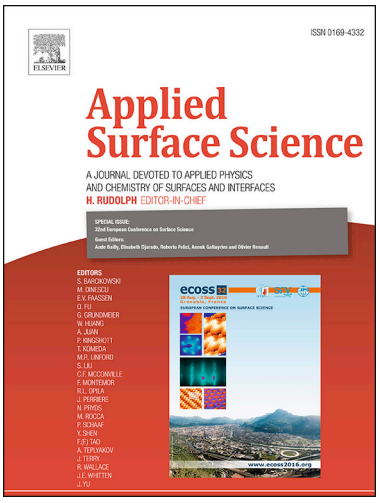

Full Length Article

A density functional based tight binding (DFTB+) study on the sulfidization-amine flotation mechanism of smithsonite

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A density functional based tight binding (DFTB+) study on the sulfidization-amine flotation mechanism of smithsonite

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Abstract: Sulfidization-amine is the most effective method for the recovery of smithsonite ($ZnCO_3$), however the interface interaction details remain unclear. The sulfidization-amine flotation mechanism of smithsonite has been studied by Density Functional based Tight Binding (DFTB+) method in this paper. The slab model of $ZnCO_3$ (101) surface was built and the adsorptions of a monolayer of OH^-, HS^- and S^{2-} ions were conducted to model the hydration effect of water and the sulfidization effect on the $ZnCO_3$ (101) surface adsorption. On the primitive smithsonite surface, the adsorption of dodecylamine (DDA) is stronger than dodecyl secondary amine (DSA) and dodecyl tertiary amine (DTA). However, DDA hardly interacts with the hydrated $ZnCO_3$ (101) surface. Under the low concentration of Na_2S, HS^- ions form a Zn-SH-SH structure on the $ZnCO_3$ (101) surface, which hinders the interaction between DDA and surface Zn atoms. Under the high concentration of Na_2S, a layer of ZnS is formed on $ZnCO_3$ (101) surface, which is favorable for the adsorption of DDA on the surface. This is consistent with the flotation practice where smithsonite flotation requires a large amount of sodium sulfide. The results could provide a microscopic investigation into the sulfidization-amine flotation mechanism of smithsonite.

Key words: Smithsonite, Flotation, DFTB+, Amine, Sulfidization

1. Introduction

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