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Density functional theory calculation of surface properties of pyrite (100) and depression of pyrite using TGA.

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Abstract content
   (Max 300 words)
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The structural relaxation, atomic Mulliken populations and electronic structures of ideal pyrite (100) surface were calculated using density functional theory (DFT). The calculated results show that the relaxation of pyrite (100) surface is relatively small, and the Fe-S interaction increases at the surface compared to that in the bulk. The calculated electronic structure results suggest that the surface 5-coordinated Fe atom has high activity. Adsorption of TGA on FeS₂ (100) surfaces is investigated, and results for CaOH⁺ and OH⁻ adsorption on FeS₂ (100) which are important in the depression process are also reported. The adsorption of thiolglycolic acid, hydroxyl and calcium hydroxyl ions (TGA, OH⁻ and CaOH⁻) on pyrite (100) surfaces was studied using first-principles calculations to investigate the depression of pyrite by TGA, NaOH and CaO. The calculation results showed that the adsorption of CaOH⁺ on pyrite surfaces was stronger than the adsorption of OH⁻ and TGA. The surface Fe atoms were the active sites for the three adsorbates. The OH obtained electrons from the surface, whereas TGA and CaOH⁺ lost electrons to the surface. The loss of electrons resulted in the accumulation of electrons on the surface, which hindered the oxidation of pyrite and the formation of dixanthogen.

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PhD

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