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Computational modelling study of pyrite surfaces and adsorption of xanthates, dithiophosphates and dithiophosphate onto pyrite.

Computational modelling methods were employed to investigate pyrite surfaces, and the effect of water molecule on the three typical thiol collectors (xanthate, dithiocarbomate and dithiophosphate) interactions at the pyrite surfaces. The calculated surface energies for {100}, {110}, {111} and {210} showed that {100} surface is most stable whereas {110} is the least stable. Morphologies of pyrite indicate predominance of the {100} facets and limited presence of others. The adsorption results suggest that the interactions of thiol collectors are via their S atoms bonding with the surface Fe atoms, indicating that the Fe atom participates in the bonding interaction. The analysis of density of states (DOS) suggest that thiol are composed of the S 3p orbital, indicating that the S 3p orbitals are very active. In addition, the DOS of S atom with a single bond is the same as the S atom with a double bond, indicating that the two S atoms in the thiol group have similar chemical reactivity, which may be ascribed to the conjugation effect of a pi bond. The presence of water molecule has an obvious effect on the electron distribution, covalent bonding and reactivity of surface atoms and consequently influences the interaction between the collector and mineral surface. These results agree well with the flotation practice.

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