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Computational and experimental study on effect of xanthate chain length on pyrite (FeS₂) mineral surfaces

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In this study ab-initio computational and microcalorimetry methods were used to study the interaction of xanthate collectors of different chain lengths on pyrite (100) and (111) surfaces. The (100) surface was found to be more stable than the (111) surface as such more dominant during ore grinding. This is also confirmed by the surface morphologies of pyrite in both approaches. Four collectors were considered, (i.e. SEX, PNPX, PNBX and PAX). The HOMO and LUMO energies computed from DMol³ revealed that the PAX had the strongest ability to donate its electrons, while SEX had the strongest ability to accept electrons. Furthermore, PAX interaction on the surfaces is the most energetically favourable collector. We also observed that the (111) surface has the strongest heat of adsorption, which is attributed to less surface stability than the (100) surface. The calculated Mulliken atomic charges showed that the xanthate collectors behaves as electron donor with the Fe atoms accept charges, forming a back donation covalent bond. The microcalorimetry test showed similar trend as the DFT adsorptions, however the heats of adsorptions were lower than DFT values. The findings depict the behaviour of xanthate of different chain length and reveal that a longer hydrocarbon chain collector may increase the floatability of the pyrite mineral.

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