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Computational and experimental studies on heats of adsorption of heterocyclic collectors onto pyrite mineral surface

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During flotation liberated particles are rendered hydrophobic by addition of organic collectors that will facilitate their attachment to air bubbles. This study employed both computational density functional theory and experimental microcalorimetry to investigate the heats of adsorption of 2-mercaptobenzothiazole (MBT), 2-mercaptobenzoxazole (MBO) and 2-mercaptobenzimidazole (MBI) onto pyrite mineral surfaces. The (100) surface was used to investigate the structural, density of states (DOS) and atomic charges to understand the reactivity of heterocyclic collectors. The selectivity of collectors to recover minerals with high grade is still a challenge and requires detailed fundamentals knowledge from both experiments and computational approaches. The heterocyclic collectors' offers hope due to their high selectivity and being able to function at neutral pH. The order or reactivity of these compounds were deduced from the predicted HOMO and LUMO energies and appears to favour MBO. We observed that the MBT adsorbed through the exocyclic sulphur atom, while MBO and MBI adsorbed through the exocyclic sulphur and N atoms onto the Fe atoms. The computed heat of adsorption energies indicated that the MBO has the strongest adsorption, and the order of reactivity decreased as: MBO > MBI > MBT for both computational and microcalorimetry. The DOS and atomic charges of the collectors indicated that the collectors S atoms behaved as electron donor, while the Fe atoms accepted charges. Computational modelling effectively predicted the reactivity of molecules and showed a great correlation with the experimental approach.

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