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Interaction of modified heterocyclic collectors with chalcopyrite mineral surface

Chalcopyrite is a major source of copper and its significance extends to a wide range of applications. Although chalcopyrite mineral recovery is achieved to some satisfactory, there is still a need to improve its recovery in particular the low grade and hard to float chalcopyrite. This requires a highly selective collector to target and float the desired mineral. The modification of collectors offers hope to enhance the performance of the collectors to have strong binding with high selectivity. The density functional theory (DFT) within the Vienna ab-initio simulation package (VASP) technique was used to modify and adsorb heterocyclic collectors such as 2-mercaptobenzothiazole (MBT), 2-mercaptobenzoxazole (MBO) and 2-mercaptobenzimidazole (MBI) by addition of an allyl group. The adsorption mechanisms showed that the collectors preferred to bind on the Cu atoms than the Fe atoms on chalcopyrite (112) mineral surface. Furthermore, the adsorption energies showed that the modified MBO gave strong adsorption (−89.42 kJ/mol). This suggested that the modified MBO may be used to enhance the recovery of chalcopyrite amongst the modified heterocyclic collectors.

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Primary author: MKHONTO, Peace (University of Limpopo)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: MKHONTO, Peace (University of Limpopo)

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