Contribution ID: **20** Type: **Poster Presentation**

COMPUTATIONAL MODELLING STUDIES ON ADSORPTION OF TRIAZINE AND XANTHATE COLLECTORS ON COOPERITE (101) SURFACES.

Cooperite has been found to have a natural floatability and therefore there are few reports on its interaction with reagents such as collectors. In this study we employed the density functional theory with dispersion correction (DFT-D) to investigate the interaction of sodium 2,6-dithio-4-butylamino-1,3,5-triazine (SDTBAT) and sodium normal butyl xanthate (SNBX) collectors with PtS (101) surface within the CASTEP code. The surface energy computed for (101) surface was found to be 1.14 J/m2. In the adsorptions, we initially tested different adsorption sites, to identify the most preferred active and exothermic site on the surface. We observed that the adsorption of SDTBAT preferred to adsorb on the 3-coordinated Pt atoms through Pt–S, Pt–N, Pt–S bridging mode. The SNBX was found to also adsorb on the 3-coordinated Pt atoms and formed a Pt–S1, Pt–S2 bridging. The SDTBAT collector was found to give the most exothermic adsorption energy of −610.1 kJ/mol compared to the SNBX which gave −378.8 kJ/mol. This indicated that SDTBAT has stronger adsorption strength than that of SNBX which suggested that SDTBAT has the potential to replace the xanthate as the collector due to its high selectivity and flotation power. Therefore this study has paved a way for design and adsorption of the triazine collectors on hard to float mineral such as sperrylite to improve their floatability.
Keywords: DFT; PtS (101) Surface; Triazine collectors; Xanthate; Adsorption energies.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

Consent on use of personal information: Abstract Submission

Primary author: Mr MANYAMA, Thato (University of Limpopo)

Co-authors: Dr MKHONTO, Peace (Universiy of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Mr MANYAMA, Thato (University of Limpopo)

Session Classification: Poster Session

Track Classification: Track G - Theoretical and Computational Physics