Contribution ID: **309** Type: **Poster Presentation**

Effects of NaOH and lime in the separation of chalcopyrite and pyrite minerals using allyl-N-diethyl dithiocarbamate as collectors: DFT and experimental studies

The separation of chalcopyrite and pyrite are usually done by taking advantage of the pH of the pulp. These are usually done by pH modifiers such as sodium hydroxide (NaOH) and lime (Ca(CO)₂) and it has been reported that these gives different recovery performance. These pH modifies have not been completely explored from the computational aspect. In this study we employed the computational density functional theory and micro-flotation to investigate the bonding mechanism of NaOH, lime and allyl-N-diethyl dithiocarbamate (ADEDTC) with reconstructed chalcopyrite (112) surface and pyrite (100) surface. We have found that lime has a strong adsorption on pyrite surface than on chalcopyrite surface, while the NaOH has strong adsorption on chalcopyrite surface than pyrite surface. The adsorption of the ADEDTC collectors gave strong adsorption on chalcopyrite and preferred the Cu atom over the Fe atoms, while the adsorption on pyrite Fe sites was weak. This was accompanied by micro-flotation recoveries, where the ADEDTC collector gave higher chalcopyrite recoveries of above 90%, and lower recoveries of pyrite. These findings provided a clear correlation between experiments with DFT predictions and also gave evidence of an adsorption of ADEDTC on Cu of chalcopyrite surface. Most importantly it has been demonstrated that lime will adsorb stronger on pyrite resulting in pyrite depression compared to NaOH during flotation. It is therefore suggested that the ADEDTC collectors and lime may be useful in floatation separation of chalcopyrite from pyrite minerals.

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

No

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

N/A

Consent on use of personal information: Abstract Submission

Primary authors: Dr MKHONTO, Peace (University of Limpopo); MKHONTO, peace prince (University of Limpopo)

Co-authors: Dr ZHANG, Xingrong (BGRIMM Technology Group); Mr LU, Liang (BGRIMM Technology Group); Dr ZHU, Yangge (BGRIMM Technology Group); Prof. HAN, Long (BGRIMM Technology Group); Prof. NGOEPE, Phuti (University of Limpopo)

Presenters: Dr MKHONTO, Peace (University of Limpopo); MKHONTO, peace prince (University of Limpopo)

Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials