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The effect of thiol collectors on nickel-rich (110) pentlandite surface

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Ab-initio density functional theory was employed to investigate the interaction of thiol collectors on the nickel-rich pentlandite Fe₄Ni₅S₈ (110) surface, in order to establish an insight into the collecting performances of SEX, SIBX and DEDTP collectors during flotation. The HOMO and LUMO energies of the three collectors were computed from DMol³ and revealed that SIBX had the strongest ability to donate electrons, while DEDTP accept electrons. We observed that the collecting strength of DEDTP on the nickel-rich pentlandite mineral (110) surface is mostly preferred amongst the three collectors. In addition, we observed that the Fe atoms had the strongest adsorption than Ni atoms. The calculated Bader charges showed that SEX and SIBX behaves as electron donor while the DEDTP as electron acceptor. This was also confirmed by the charge density difference, which showed charge accumulation on metals and charge depletion on S atoms of the collectors. Interestingly, we observed a charge accumulation at the internuclear region between the adsorbed metal and S atoms of collector. This indicated that some charges are localised in this region forming a normal covalent bond for DEDTP and back donation covalent bond for SEX and SIBX. The PDOS for the adsorbed system showed that the 3p-orbital HOMO peak is reduced near the EF, suggesting a strong interaction between the S of collectors and the Fe/Ni atoms.

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Phuti E. Ngoepe
phuti.ngoepe@ul.ac.za
University of Limpopo

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Primary author: Dr MKHONTO, Peace (University of Limpopo)

Co-author: Prof. CHAUKE, Hasani (University of Limpopo)

Presenter: Dr MKHONTO, Peace (University of Limpopo)

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