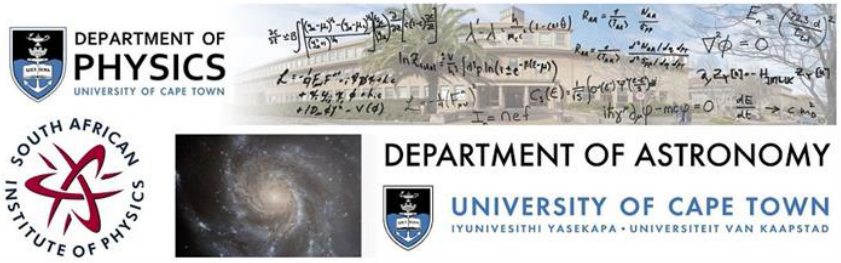

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Interactions of xanthates and dithiophosphate on (110) nickel-rich pentlandite (Fe₄Ni₅S₈) mineral surface

Tuesday, 5 July 2016 14:00 (20 minutes)

Abstract content
   (Max 300 words)
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Ab-initio density functional theory was employed to investigate the adsorption of sodium ethyl xanthate (SEX), sodium isobutyl xanthate (SIBX) and diethyl dithiophosphate (DEDTP) collectors on the nickel-rich pentlandite Fe₄Ni₅S₈ (110) surface. Two adsorption sites have been considered; the Ni-top and Fe-top sites. The electron density of the clean (110) surface is found to be high on Ni atoms than on Fe atoms suggesting a strong covalent bonding. Furthermore, the results show that the adsorbates coordinate mainly to the surface through interaction between their S atoms with the surface Fe or Ni atoms; the sulphur atoms of these thiol collectors being the centre of reactivity. The adsorption energies showed that DEDTP adsorbs stronger than the xanthates, and the predicted adsorption strength follows the order as: DEDTP > SIBX > SEX for both Ni-top and Fe-top sites. The DOS and Bader charge analysis suggest that the xanthates act as electron donors while the DEDTP has an electron accepting character at the surface. These properties suggest that the DEDTP exhibit good selectivity in the separation of pentlandites as compared to SIBX and SEX xanthates. This study offers an insight into the collecting performance of SEX, SIBX and DEDTP on (110) nickel-rich pentlandite mineral surface, which could guide recovery operations.

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