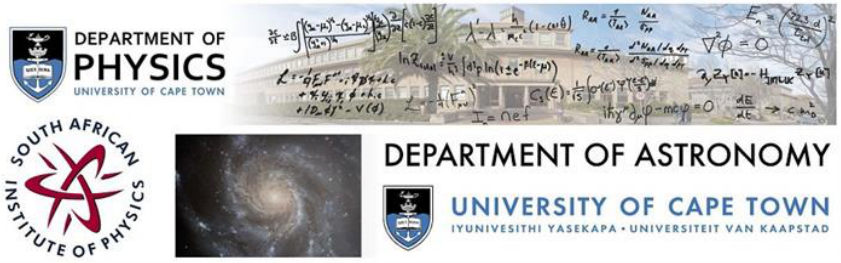

Contribution ID: **502** Type: **Oral Presentation**

Modelling of Pyrite (FeS₂) surfaces and adsorption of dithiophosphate (DTP) onto pyrite surface.

Wednesday, 6 July 2016 14:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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Computational modelling methods were employed to investigate pyrite surfaces, and the adsorption of DTP on pyrite surface. The calculated surface energies for {100}, {110}, {111} and {210} showed that {100} surface is most stable whereas {110} is the least stable. Morphologies of pyrite indicate predominance of the {100} facets and limited presence of others. The adsorption results suggest that the interactions of DTP collectors are via their S atoms bonding with the surface Fe atoms, indicating that the Fe atom participates in the bonding interaction.

The analysis of density of states suggest that DTPs are composed of the S 3p orbital, indicating that the S 3p orbital are very active. In addition, the density of states of the S atom with a single bond is the same as the S atom with a double bond, indicating that the two S atoms in the thiol group have similar chemical reactivity, which may be ascribed to the conjugation effect of a pi bond.

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