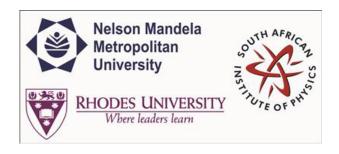
## **SAIP2015**



Contribution ID: 154 Type: Oral Presentation

## First principle study of Xanthate and Diethyldithiophosphate adsorption on PtS (010) surface

Tuesday, 30 June 2015 14:20 (20 minutes)

Abstract content <br/> &nbsp; (Max 300 words)<br/> dry-<a href="http://events.saip.org.za/getFile.py/atarget="\_blank">Formatting &<br/> &class="blank">Formatting &class="blan

Platinum surface has been studied extensively in recent years to improve the fundamental understanding of the mechanism of oxidation reaction on metal surfaces. These surfaces have a wide scientific and technological interest, particularly because of their catalytic properties. Density functional theory (DFT) method has been employed to study the surface properties of Platinum sulphide mineral PtS (010) and their interaction with xanthate and diethyldithiophosphate. It was noted that the adsorption energy of SEX is more exothermic compared to EX and IBX is more exothermic compared to SIBX. Furthermore, the adsorption energy of DEDTP shows that it is high in selectivity.

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**Primary author:** Ms MASENYA, Mamogo (University of Limpopo)

**Presenter:** Ms MASENYA, Mamogo (University of Limpopo)

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