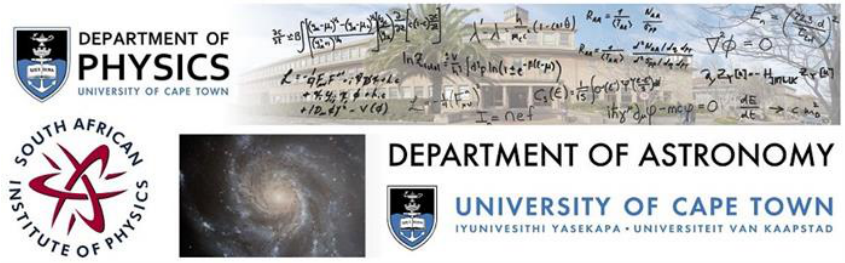

Contribution ID: **143** Type: **Poster Presentation**

Density functional theory study of PtS surfaces

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Precious metal sulphides such as PtS and PdS are major compounds occurring in the Pt and Pd ores, and play an important role as catalyst in the petroleum refining industry. In our previous work, the PtS and PdS minerals were investigated using density functional methods within planewave pseudopotential methods and predicted stability of PtS, Pt_{12.5}Pd_{37.5}S₅₀ and PdS phases. The current study is based on the surface properties of PtS and their interaction with oxygen and water molecules. It was found that the (010) surface displayed the lowest energy, hence is the most stable. Furthermore, it was observed that the sodium isobutyl xanthate (SIBX) adsorbs stronger on the surface compared to sodium ethyl xanthate (SEX).

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

Yes

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

MSc

Main supervisor (name and email)
and his / her institution

P.E. Ngoepe, Phuti.Ngoepe@ul.ac.za
University of Limpopo

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Please indicate whether
this abstract may be
published online
(Yes / No)

No

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

Presenter: Ms MASENYA, Mamogo (University of Limpopo)

Session Classification: Poster Session (1)

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