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## Density functional theory study of PtS surfaces

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

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<sub>12.5</sub>Pd<sub>37.5</sub>S<sub>50</sub> 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).

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