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## **Ab-initio studies of sperrylite, platarsite and palladoarsenide phase stability and surfaces**

Thursday, 11 July 2019 15:00 (2 hours)

Computational modelling studies of platinum group minerals (PGM): sperrylite ( $\text{PtAs}_2$ ), platarsite ( $\text{PtAsS}$ ) and palladoarsenide ( $\text{Pd}_2\text{As}$ ), were carried out to investigate their stabilities and surfaces. These are paramount to the mining industry in South Africa as they are the most extracted minerals in the Platreef bushveld complex. In this study we employed the Vienna *Ab-initio* Simulation Package (VASP) along with the projector augmented wave (PAW) method to investigate the structural stability and surface stabilities of  $\text{PtAs}_2$ ,  $\text{PtAsS}$  and  $\text{Pd}_2\text{As}$ . In addition, the phase stability of  $\text{PtAsS}$  was investigated using cluster expansion, while the  $\text{PtAs}_2$  and  $\text{Pd}_2\text{As}$  were obtained from phonon dispersions. We found that the calculated lattice parameters of the studied structures are in good agreement with the experimental data. The  $\text{PtAsS}$  cluster expansion showed that all generated structures are thermodynamically stable and the phonon showed no soft modes for  $\text{PtAs}_2$ ,  $\text{PtAsS}$  and  $\text{Pd}_2\text{As}$  structures. The calculated surface energies indicated that the (100) surface for  $\text{PtAs}_2$ ,  $\text{PtAsS}$  and  $\text{Pd}_2\text{As}$  was the most stable amongst the low miller index (100), (110) and (111) surfaces. As such the (100) surface was considered as the working surface for all the surface models. The order of surface energies followed as: (100) < (111) < (110) for  $\text{PtAs}_2$  and  $\text{PtAsS}$  and (100) < (110) < (111) for  $\text{Pd}_2\text{As}$ . The calculated thermodynamical equilibrium morphologies of the relaxed surface structures indicated that (100) surface was the most dominate surface for all the studied surface structures. These findings gave more insights on the stability of these minerals and their surface stabilities which may be applicable in their recovery.

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

Yes

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

MSc

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