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

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Computational modelling studies of platinum group minerals (PGM): sperrylite (PtAs₂), platarsite (PtAsS) and palladoarsenide (Pd₂As), were carried out to investigatate 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 PtAs₂, PtAsS and Pd₂As. In addition, the phase stability of PtAsS was investigated using cluster expansion, while the PtAs₂ and Pd₂As 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 PtAsS cluster expansion showed that all generated structures are thermodynamically stable and the phonon showed no soft modes for PtAs₂, PtAsS and Pd₂As structures. The calculated surface energies indicated that the (100) surface for PtAs₂, PtAsS and Pd₂As 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 PtAs₂ and PtAsS and (100) < (110) < (111) for Pd₂As. 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.

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Yes

Level for award
 (Hons, MSc,
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MSc

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