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Ab initio study of the structural, mechanical and electronic properties of PtAs2, PtAsS and Pd2As minerals

The PGMs are predominantly found in the Platreef Bushveld Complex, and the most common are Pt in the form of sperrylite (PtAs2), platarsite (PtAsS) and Pd found in the form of palladoarsenide (Pd2As) minerals. The investigations of the structural, mechanical and electronic properties of PtAs2, PtAsS and Pd2As were accomplished by employing Vienna Ab-initio Simulation Package (VASP) code at Lengau cluster, using 48 cores for two days. We found that the calculated lattice parameters are in excellent agreement with the available experimental data. In addition, the calculated heats of formation predicted that PtAs2 was more stable. The computed elastic constants showed that they are mechanically stable and the phonon dispersion curves showed no soft modes for PtAs2, PtAsS and Pd2As, suggesting stability. We observed that the Pd2As and PtAsS were of ductile, while PtAs2 is brittle. The calculated total density of states (TDOS) for the bulk PtAsS and Pd2As showed a metallic behaviour since there is no band gap at the Fermi energy (EF). The PtAs2 was observed as a semiconductor with an indirect gap of 0.104 eV. From the DOS, the PtAs2 was found the most stable since it had less contribution of density of states at the EF, while PtAsS and Pd2As showed least stability due to highest density of states at the EF. These findings gave more insights on the stability of these minerals which may be applicable to their recovery.

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