Contribution ID: **131**   Type: **Poster Presentation**

Investigation of the structural, elastic and vibrational stability of PtTe, PtTe2, Pt2Te3 and Pt3Te4 tellurides structures

Tuesday, 4 July 2023 16:05 (1 minute)

Platinum tellurides are platinum group minerals (PGMs) predominantly found in the Platreef Bushveld Complex of South Africa, which is one of the leading countries with highest percentages of PGMs. Besides being the important carriers of precious metals, telluride minerals are minor constituents in an ore deposits from a wide diversity of geological environments and they are of significant economic importance. In this study Vienna Ab-initio Simulation Package (VASP) code was employed to investigate the structural, thermodynamic, elastic and vibrational properties of PtTe, PtTe2, Pt2Te3 and Pt3Te4.The calculated lattice parameters agreed well with the available experimental data. In addition, the calculated heats of formation predicted that PtTe2 was more stable than the PtTe, Pt2Te3 and Pt3Te4. The elastic constants indicated that PtTe, PtTe2, Pt2Te3 and Pt3Te4 were mechanically stable. It was observed that the PtTe was ductile, while PtTe2, Pt2Te3 and Pt3Te4 were brittle. The phonon dispersion curves showed no soft modes for PtTe, PtTe2 and Pt3Te4 suggesting stability, while Pt2Te3 was unstable due to the presence of vibrations in the negative frequency. The total density of states (TDOS) for all the structures showed a metallic behaviour due to absence of a band gap. These findings gave more insights on the stability of these minerals for future studies that will include surfaces in particular for PtTe2 which is dominates in the Platreef Bushveld Complex.

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HONS

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Presenter: MAAKA, TSHEPO

Session Classification: Poster Session 1

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