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Computational Modelling Studies of Platinum Telluride Minerals

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Abstract content
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Besides being the important carriers of precious metals, telluride minerals are minor constituents in an ore deposits from a wide diversity of geological environments. In spite of the fact that these telluride minerals are of significant economic importance, not much has been done on their recovery. In this work density functional theory (DFT) method was employed to study the structural, energetic, electronic and mechanical properties of the PtTe₂ structure. In addition, the low Miller index {100}, {110} and {111} for PtTe₂ mineral were investigated. The calculated lattice constants of PtTe₂ structure are in a good agreement with the experimental data. The elastic properties satisfied all necessary conditions for mechanical stability. The surface {100} was found to be stable since it gave the lowest positive surface energy.

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Main supervisor (name and email)
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