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Investigation of Structural and Dynamical Properties of Sperrylite (PtAs2) Mineral Based on Molecular Dynamics Simulations

The precious metals are extracted as valuable by-products from sulphides and arsenides- platinum group minerals (PGMs). The growing use of precious metals in the mineral processing industry has developed a deep interest in extracting them from the PGMs. In this study, computational modelling technique, molecular dynamics (MD) is applied to investigate structural and physical properties of sperrylite (PtAs2). The derived and validated Interatomic potentials for MD simulations will be used. Radial distribution functions (RDFs) and mean square displacement (MSD) are used to establish the effect of temperature and pressure on the sperrylite mineral. Simulation details, such as the convergence of results on the simulation time and transport properties, are also discussed. The understanding of the structural and dynamical properties of sperrylite mineral under extreme conditions could pave the way for research on the behaviour of arsenic-containing minerals and sulphide minerals.

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

Yes

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

MSc

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