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An Atomistic Simulation Study of Arsenopyrite (FeAsS) and Sperrylite (PtAs2) Minerals

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. The structure and thermodynamic properties of arsenopyrite (FeAsS) and sperrylite (PtAs2) must be better understood in order to extract the precious metals from the ores effectively. In this study, the general utility lattice program (GULP) code was used to derive the new interatomic potentials of FeAsS and PtAs2. The interatomic potentials of FeAsS were obtained, for the first time and the available interatomic potentials of PtAs2 that were previously found to give stiff material property were refined. The novelty of these interatomic potentials in terms of the elastic constants and bulk modulus were in good agreement with the ab-initio density functional theory (DFT) results and experimental data was scarce.

Student?

Yes

Supervisor name

Dr Mofuti Mehlape

Supervisor email

mofuti.mehlape@ul.ac.za

Primary author: NTOBENG, Thapelo (University of Limpopo)

Co-authors: MEHLAPE, Mofuti (University of Limpopo); MKHONTO, Peace (university of Limpopo); NGOEPE, Phuti (University of Limpopo)

Presenter: NTOBENG, Thapelo (University of Limpopo)

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