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## Investigate the bulk and surfaces properties of PtAs<sub>2</sub>, PtSb<sub>2</sub> and PtBi<sub>2</sub> PGMs using the Ab-Initio Molecular Dynamics (AIMD) with Machine Learned Force Fields (MLFF) technique

### Abstract

The currently available machine learned force-field (MLFF) within ab-initio molecular dynamics (AIMD) embedded with the Vienna ab-initio simulation package (VASP), allows for generation of force field to handle large systems. The AIMD-MLFF methods were employed in the current study to investigate the bulk and surface properties of sperrylite (PtAs<sub>2</sub>), geversite (PtSb<sub>2</sub>) and insizwaite (PtBi<sub>2</sub>) platinum group minerals (PGMs) at 300 K. After training the lattice parameters were obtained as: PtAs<sub>2</sub> (5.977 Å), PtSb<sub>2</sub> (6.457 Å) and PtBi<sub>2</sub> (6.721 Å). The trained force fields were then applied on 4x4x4 supercell produced lattice parameters of: PtAs<sub>2</sub> (5.991 Å), PtSb<sub>2</sub> (5.445 Å) and PtBi<sub>2</sub> (6.723 Å). These were found to be in good agreement with the experimental values of 5.970 Å, 6.440 Å and 6.702 Å for PtAs<sub>2</sub>, PtSb<sub>2</sub> and PtBi<sub>2</sub>, respectively. From ab-initio the (100) surfaces was determined as the most stable surface for all three minerals with PtAs<sub>2</sub> having the surface of (1.00 J/m<sup>2</sup>), PtSb<sub>2</sub> (0.42 J/m<sup>2</sup>) and PtBi<sub>2</sub> (0.15 J/m<sup>2</sup>). The trained (100) surfaces for all minerals gave surface energies of: PtAs<sub>2</sub> (1.76 J/m<sup>2</sup>), PtSb<sub>2</sub> (1.32 J/m<sup>2</sup>) and PtBi<sub>2</sub> (0.97 J/m<sup>2</sup>). Again, trained force fields applied to supercell (100) surfaces yielded surface energies of PtAs<sub>2</sub> (1.67 J/m<sup>2</sup>), PtSb<sub>2</sub> (1.27 J/m<sup>2</sup>), and PtBi<sub>2</sub> (1.93 J/m<sup>2</sup>). These demonstrated that the viability of the AIMD-MLFF method at 300 K, produces results that correlate with experiment and ab-initio results. This cleared the path for the potential application of such a machine learning technique to surface adsorption.

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