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Investigate the bulk and surfaces properties of PtAs2, PtSb2 and PtBi2 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 (PtAs2), geversite (PtSb2) and insizwaite (PtBi2) platinum group minerals (PGMs) at 300 K. After training the lattice parameters were obtained as: PtAs2 (5.977 Å), PtSb2 (6.457 Å) and PtBi2 (6.721 Å). The trained force fields were then applied on 4x4x4 supercell produced lattice parameters of: PtAs2 (5.991 Å), PtSb2 (5.445 Å) and PtBi2 (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 PtAs2, PtSb2 and PtBi2, respectively. From ab-initio the (100) surfaces was determined as the most stable surface for all three minerals with PtAs2 having the surface of (1.00 J/m2), PtSb2 (0.42 J/m2) and PtBi2 (0.15 J/m2). The trained (100) surfaces for all minerals gave surface energies of: PtAs2 (1.76 J/m2), PtSb2 (1.32 J/m2) and PtBi2 (0.97 J/m2). Again, trained force fields applied to supercell (100) surfaces yielded surface energies of PtAs2 (1.67 J/m2), PtSb2 (1.27 J/m2), and PtBi2 (1.93 J/m2). 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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