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Exploring the bulk and surface structures of ZnS, FeS2 and PbS minerals using AIMD-MLFF technique.

Sphalerite (ZnS), pyrite (FeS₂), and galena (PbS) are found in association with each other in the mineral's ore deposits. The separation of these minerals is critical and these require fundamental understanding from the surface properties. The study investigated the behaviour of the surface properties of these minerals at room temperature (300 K) utilizing the ab-initio molecular dynamic (AIMD) with machine learned force fields (MLFF) methods in comparison with the standard ab-initio simulations. The methods are integrated into the Vienna Ab Initio Simulation Package (VASP) code. The MLFF training of the bulk unit cells generated the force fields which were applied on the 4x4x4 supercells of ZnS, FeS₂ and PbS and produced lattice parameters of 5.405 Å, 5.420 Å and 6.014 Å, respectively. These were in good agreement with the experimental values of 5.410 Å, 5.419 Å and 5.999 Å, respectively. The most stable surfaces were cleaved and the surface energies for ZnS (110), FeS₂ (100) and PbS (100) surfaces were computed from the training and from the force fields generated. It was found that the surface energies ZnS (0.71 J/m²), FeS₂ (1.66 J/m²) and PbS (0.73 J/m²) were in good agreement with those obtained from the standard ab-initio calculations ZnS (0.68 J/m²), FeS₂ (1.32 J/m²) and PbS (1.11 J/m²). These surface energies suggested that pyrite is harder than the sphalerite and galena, which indicated that the grinding of the ore with these minerals may require more time for fine griding of pyrite compared to sphalerite and galena.
 Keywords: VASP code; AIMD-MLFF; Surface energies; lattice parameters; ZnS (110); FeS₂ (100) and PbS (100).

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Primary author: Mr MANYAMA, Thato (University of Limpopo)

Co-authors: MKHONTO, Peace (University of Limpopo); NGOEPE, Phuti Esrom (University of LImpopo)

Presenter: Mr MANYAMA, Thato (University of Limpopo)

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