



Contribution ID: 99

Type: Poster Presentation

Computational modelling studies of oxidation and hydration on NiS₂ and NiAs₂ surfaces

Tuesday, 26 June 2018 15:00 (2 hours)

The atmospheric oxidation of minerals either by weathering or aging involves physical and chemical adsorption of oxygen on the surfaces and this forms various peroxides and hydroxides. In this study a *ab-initio* computational method was employed to investigate the interaction of oxygen and water molecules at different adsorption sites on the most stable surfaces of NiS₂ and NiAs₂. Their calculated surface energies showed that the NiS₂ (100) and NiAs₂ (111) surfaces are more stable. We predicted the order of surface stability as: (100) > (111) > (210) > (110) for NiS₂ and (111) > (110) > (100) > (210) for NiAs₂. The adsorption of O₂ was found to dissociate on mineral surfaces and different bonding mechanisms of the oxygen atoms were depicted. The O₂ adsorption on both NiS₂ (100) and NiAs₂ (111) surfaces was exothermic with adsorption energies of -3.19 eV and -4.83 eV, respectively. The H₂O adsorption on both NiS₂ (100) and NiAs₂ (111) mineral surfaces were found to relax deep into the surface. The H₂O adsorption on Ni-top site was more exothermic, suggesting preferential adsorption on Ni atoms than on S and As atoms on both NiS₂ and NiAs₂. These investigations suggests that the oxidation of NiS₂ and NiAs₂ prefer adsorbing on S and As atoms than on Ni, while the hydration of NiS₂ and NiAs₂ prefer adsorbing on Ni atoms than S and As atoms. These investigations provide information on the bonding mechanism and chemistry of oxygen and water molecules onto NiS₂ (100) and NiAs₂ (111) surfaces that may be applicable to the atmospheric oxidation and during flotation process or mineral extraction.

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Session Classification: Poster Session 1

Track Classification: Track A - Physics of Condensed Matter and Materials