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

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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 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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