



Contribution ID: 213

Type: **Poster Presentation**

Density Functional Study on the adsorption of O₂ and H₂O on PtSb₂ (100) surface.

The interactions of O₂ and H₂O with mineral surfaces are the major factors that determine the oxidation and wettability behaviour of minerals. This study employed the first-principles density functional theory to explore the bonding behaviour, adsorption energies and electronic properties directly related to the reactivity of O₂ and H₂O with geversite (100) mineral surface. The oxidation of the surface resulted in formation of superoxide, peroxide and bridging adsorption, where the peroxide adsorption on Pt atom was more exothermic (-64.29 kJ/mol). The hydration showed that both Pt and Sb atoms interact with water through oxygen atom. However, under multi water adsorption (-38.19 kJ/mol), the water molecule flipped hydrogen down and consequently interacts with the surface through hydrogen atoms. In comparison of adsorption energies of the O₂ and H₂O, we found that oxidation was more exothermic than the hydration, which suggest a preferential oxidation of the geversite mineral. This study provides insights on the hydration and oxidation of geversite that may be applicable in the recovery processes.

Apply to be considered for a student ; award (Yes / No)?

no

Level for award;(Hons, MSc, PhD, N/A)?

N/A

Primary authors: MANGWEJANE, Samuel Seshupo (University of Limpopo); Dr MKHONTO, Peace (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: MANGWEJANE, Samuel Seshupo (University of Limpopo)

Session Classification: Theoretical and Computational Physics

Track Classification: Track G - Theoretical and Computational Physics