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

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Session Classification: Theoretical and Computational Physics

Track Classification: Track G - Theoretical and Computational Physics