Contribution ID: **305** Type: **Poster Presentation**

Computer Simulation Study of Synthetic Nickel-Rich Pentlandite (Fe₄Ni₅S₈) Surfaces

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Abstract content
   (Max 300 words)

Density Functional Theory (DFT) with the plane-wave (PW) pseudo-potential method within the VASP code is employed to investigate the interaction of oxygen and water molecules on the synthetic nickel-rich pentlandite {100} and {110} surfaces. The oxygen-metal interaction show preferential iron oxidation than nickel on both surface models. However, a bridging of the oxygen molecule between the Fe-Ni metals on the {100} surface prefers the horizontal orientation with strong adsorption energy of -5.60 eV, while the un-oxidized nickel atoms dissociates into the sub-surface. We also observe a peroxo isomer anion (Fe (O₂) ⁻) species on the {100} surface with one oxygen forming a bridging bond with the nearest nickel atom. Moreover, the iron preferential oxidation is clearly seen on the {110} surface with the vertical orientation, where it moves towards iron forming a bridge. The oxidation of the nickel atom showed the presence of superoxo isomer species on the {110} surface. The hydration of nickel on {100} surface gives the most stable surface compared to {110} with a strong adsorption energy of -2.96 eV (exothermic) and while endothermic process is observed for the {110} surface (0.14 eV). However, hydration of {110} surface, in particular on the iron atom shows weak adsorption energy -0.07 eV (exothermic).

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yes

Level for award
 (Hons, MSc,
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MSc

Main supervisor (name and email)
and his / her institution

Prof P.E Ngoepe, phuti.ngoepe@ul.ac.za, University of Limpopo

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Primary author: Mr MKHONTO, Peace Prince (University of Limpopo)

Presenter: Mr MKHONTO, Peace Prince (University of Limpopo)

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