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Computational Modelling Study of nickel-rich pentlandite {111} surface

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Abstract content
 (Max 300 words)

<i>Ab-initio</i> density functional theory was employed to investigate the interaction of oxygen, water and ligands molecules on the nickel-rich pentlandite Fe₄Ni₅S₈ {111} surface. Pentlandite is the major source of the world's suppliers of nickel. In this study, we focus on the oxidation, hydration and addition of collectors on the nickel-rich pentlandite mineral. During adsorption, we observe that the oxygen-metal interaction showed preferential iron oxidation than nickel on the surface. Moreover, the iron preferential oxidation is extensively observed when O₂ is adsorbed on nickel. The oxidation of the iron atom showed the presence of superoxo isomer species on the surface, while the migration of the oxygen molecule from nickel to iron shows a peroxo species. The hydration on iron-nickel surface termination show that the water molecule migrate from nickel atom to bond with iron, suggesting that more water is required on the surface to hydrate the nickel atoms. Deposition of sodium ethyl xanthate (SEX) ligand on the surface enhances the bridging interaction, the iron-SEX-nickel.

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

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

Co-authors: Prof. CHAUKE, Hasani Richard (University of Limpopo); Prof. NGOEPE, Phuti E. (University of Limpopo)

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

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