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Computational modelling study of hydrated nickel-rich pentlandite (110) surface

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The hydration of minerals is one of the main processes that occur during mineral processing. These include wet grinding of the ore and during flotation of liberated particles. In this study we employed ab-initio density functional theory to investigate the adsorption of water molecules onto nickel-rich pentlandite (110) surface. We considered three adsorption aspects: Fe-top, Ni-top and complete surface coverage adsorptions and explored the bonding geometry, density of states (DOS) and Bader charges which are directly related to the reactivity of the water molecules. The hydrophobicity and hydrophilicity of minerals during mineral processing require detailed understanding in the mineral-water interaction that could give valuable insight during flotation. We found that the adsorption of water molecules on pentlandite (110) surface showed exothermic reaction. The water adsorption energies were more exothermic on Fe-top than Ni-top. This indicates that the water molecule interacts strongly with Fe than Ni atoms. The complete surface coverage revealed a physisorption process on (110) surface. Furthermore, DOS showed orbital shift to lower energy level and their energy states are lowered near E_F. This indicates that there are electron/charge transfers from the surface metals to the water molecule. The charge density difference indicated that some charges are localised at the internuclear region. Due to the 1b₁-3d orbital mixing, some charges are depleted from the 3d-orbitals to the lower lying manifold 3d-orbitals. These observations gave valuable insights on how the metals (Fe and Ni) react with water during mineral extraction using the flotation process.

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