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Computational modelling studies of Pentlandite (Fe, Ni)9S8 surface: Oxidation and hydration

Minerals are exposed to oxidation due to weathering and aging which have significant effect on their floatation. Furthermore, the hydrophobicity and hydrophilicity of minerals are crucial in determining their wettability that can be useful in the floatation process design. In this study we investigate the structural, surface and electronic properties of the nickel-rich pentlandite (Fe4Ni5S8) and the bonding and electronic structure of (111) surface oxidation and hydration. We employed computational modelling technique; the density functional theory (DFT). CASTEP code was used to investigate the oxidation and hydration reaction on nickel-rich pentlandite (111) surface. The oxidation resulted in metal preferential bonding and formation of Ni-Peroxide (-262.41 kJ/mol), which resulted from the bridging (Fe-O2-Ni) was observed to be more exothermic. For the hydration we noted strong exothermic interaction of H2O with Fe (-52.9233 kJ/mol) than Ni (-21.4832 kJ/mol) on pentlandite (111) surface and it indicated that water adsorb on the pentlandite surface through the Fe atoms. The computed density of states (DOS) for the most stable exothermic adsorption sites displayed a transition of the EF to the pseudo gap for Fe atoms, suggesting stability. We further observed that the oxygen molecule accept electrons from both Fe and Ni atoms. The hydration also displayed the oxygen and hydrogen peak to move to the valance band indicating electron acceptor from the Fe atom. This study predict the oxidation and hydration of pentlandite mineral that may be applicable in their recovery.

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

Yes

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

Hons

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