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Computer simulation study of water adsorption on {110} surface of nickel-rich pentlandite (Fe₄Ni₅S₈) mineral

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Abstract content
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Pentlandite (Co,Fe,Ni)₉S₈ is the most abundant iron-nickel sulphide ore containing mineral and has a wide range of applications in industries. The mineral is of commercial importance and can be extracted using floatation processes. Ab-initio density functional theory was employed to investigate the interaction of water on the nickel-rich pentlandite (Fe₄Ni₅S₈) {110} surface, to understand the adsorption behaviour on the ore mineral surface during ore grinding and during flotation. We considered three adsorption trajectories, i.e. Ni-top, Fe-top and complete surface coverage. It was observed that the hydration on iron-nickel surface termination shows a strong interaction of the water molecule with the iron atom. We found adsorption energy of -0.117 eV for Ni-top site adsorption and -0.320 eV for Fe-top site adsorption, while the complete surface coverage showed adsorption energy of -0.212 eV. This suggested that physisorption behaviour is favourable confirming a domination of Van Der Waal interactions. Furthermore, the PDOS plot projected onto the O s- and p-orbitals; and H s-orbitals for the H₂O molecule adsorbed on Ni and Fe atoms, show water orbitals shift to lower energy compared to the isolated water molecule. This energy shift is an indication of strong interactions with the surface Ni3b and Fe1 atoms. As such an electron gain on the oxygen atoms of the water molecule is noted. The charge transfer from the Fe/Ni atoms to the oxygen molecule of the water molecule is described using Bader analysis and charge density difference which showed a poor charge transfer of the Fe and Ni atoms.

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