Adsorption and Wetting Behavior of Epidote in Hematite Flotation: Insights from Experiments and Atomistic Simulations

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Froth flotation is a key beneficiation method in iron ore processing. Particularly, it is used in the flotation of hematite ore for removal of gangue (not valuable) minerals such as quartz (SiO_2), dolomite ($CaMg(Co_3)_2$), and epidote ($Ca_2Al_{2.16}Fe_{0.84}Si_3O_{12}(OH)$). Among these, dolomite and epidote present significant challenges for the application of starch – the most common depressant for hematite (Fe_2O_3). The main problem arises from the adsorption of starch on dolomite (primarily at Ca and Mg sites) and epidote (likely at Ca and Fe sites). Each mineral exhibits different adsorption affinity and mechanisms depending on their specific surface chemistry. To address this challenge, it is important to understand the adsorption mechanisms of reagents, such as starch and other depressants, within the flotation cell, specifically focusing on how they interact with or adsorb onto mineral surface during the process.
In this study, we combine experimental and theoretical approaches to investigate the complex interactions on epidote surfaces. The experimental work included hydrophobicity tests, and surface characterization via microscopy and spectroscopy. In the theoretical part, we calculated and compared the adsorption energies of a single water molecule (H_2O), hydroxyl (OH^-), and starch on the (100), (010), and (001) planes of epidote ($Ca_2Al_2FeSi_3O_{12}(OH)$) using density functional theory (DFT) study. Additionally, we compared computational and experimental water contact angles using Molecular Dynamics (MD) simulations. Furthermore, we performed MD simulations using systems that mimic an actual flotation cell to understand the interfacial interactions occurring within realistic flotation environment.
This research aims to provide new insights into the molecular-scale mechanisms governing epidote behavior in flotation systems. Ultimately, this work elucidates the mechanisms required for the effectively removal of epidote, supporting more efficient removal of epidote in iron ore beneficiation.

Keywords:
flotation, molecular dynamics simulations, hydrophobicity, interface