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Structural properties of the hematite and dolomite surfaces – towards the flotation separation.

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Flotation is widely used in the mining industry to separate valuable or desired minerals from gangue (undesired) minerals. This process is extensively employed in the treatment of iron ore. Therefore, separating gangue minerals (dolomite and magnesite) from iron oxide minerals (hematite) is a crucial field of study, with emphasis on dolomite and hematite since they are prevalent in the region of the Minas Gerais and their separation processes are underexplored.

To establish the most favorable cleavage directions and the surfaces is the first step to understand the differences of the hematite and dolomite surfaces with respect to the adsorption of collectors such as starch-diol-lauric, starch-diol-oleic and oleic alcohol. The difference in the geometrical and electronic structure of the surfaces and characterize the adsorption sites are explored.

We used Density Functional (DFT) calculations as implemented in the Quantum Espresso software [1] to optimize the dolomite and hematite structures. Variations in cutoff energies and k-point meshes were performed to determine convergence criteria, calculation accuracy, and computational efficiency. The cutoff energy values for hematite and dolomite were set at 60 Ry, with k-point values of 4 4 2 and 3 3 1, respectively. The optimized structures are depicted in **Figure 1**. The calculated lattice parameters for the hematite cell are **a**=**b**=5.727Å **c**=14.849Å and for dolomite **a**=**b**=4.843Å **c**=16.052Å must be compared to the experimental values **a**=**b**=5,0380 Å **c**=13,7720 Å (hematite) and **a**=**b**= 4.796Å, and **c**= 15.974Å (dolomite).

The comparison of the cleavage and surface energies of hematite and dolomite will be presented and discussed along the adsorption energy of the collector in the different surfaces.

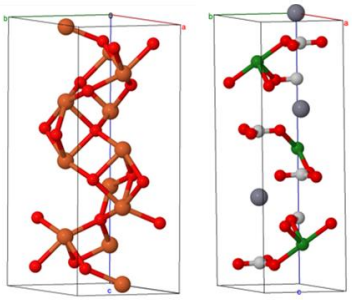

Figure 1: Optimized structures hematite (left) and Dolomite (right). The atoms of (Fe) are represented in orange, (O) in red, (Ca) in blue, (C) in gray, and (Mg) in green.

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References

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