Adsorption of H_4SiO_4 as a Hydrolysate of Sodium Silicate on Surfaces of Fluorite (111), Calcite (104), and Scheelite (112): a Density Functional Theory Approach

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H_4SiO_4 , a hydrolysate of sodium silicate, is the important species in the adsorption process during flotation separation. In this work, the interaction mechanism and adsorption behavior in the surface-chemistry of H_4SiO_4 molecule on the most stable surfaces of three calcium minerals, fluorite (111), calcite (104), and scheelite (112), were investigated systemically by using ab-initio calculation because the lack experimental approaches at the atomistic level. The results indicated that electrostatic interactions occurred between the electronegative oxygen atom of the H_4SiO_4 molecule and a calcium atom on the mineral surfaces, hydrogen bonds was observed between the hydrogen atoms of the H_4SiO_4 molecule and an oxygen atom or a fluorine atom of the calcium mineral surface, and the OH groups of H_4SiO_4 were significantly stretched during adsorption. The adsorption energy of H_4SiO_4 molecule on the surfaces of fluorite (111), calcite (104), and scheelite (112) were -1.72, -1.21, -1.55 eV, respectively. Hence, fluorite and calcite were the most and the least sensitive mineral to the adsorption of H_4SiO_4 during flotation separation, respectively. The electronic structure show that the chemisorption of H_4SiO_4 molecules on the surfaces of calcium minerals could change electron distribution and the overlaps between Ca-3p and O-2s orbitals and Ca-3d and O-2p orbitals, which led to the formation of new O-Ca bonds.

Keywords: H_4SiO_4 ; adsorption; calcium minerals; DFT

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