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Surface and Flotation Characteristics of Spodumene: A Molecular Modeling Approach

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Surface characteristics of spodumene [$LiAl(SiO_3)_2$] and aluminosilicates (feldspar [$KAlSi_3O_8$] and muscovite [$K_2Al_4(Al_2Si_6O_{20})(OH)_4$]) are modeled using molecular simulations. Surface energies are computed for various cleavage planes of these minerals and compared with those measured experimentally. Adsorption mechanisms of oleate collector on spodumene in the selective flotation of spodumene from these aluminosilicates are studied using molecular modeling methods. Further, the wettability characteristics of spodumene are quantified by computing the contact angle of a drop of water on the adsorbed oleate layer. These simulated computed contact angles are compared with those measured experimentally.