Surface and Flotation Characteristics of Spodumene:
A Molecular Modeling Approach

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Surface characteristics of spodumene \([\text{LiAl(SiO}_3\text{)}\text{]}\) and aluminosilicates (feldspar \([\text{KAISi}_3\text{O}_8]\)
and muscovite \([\text{K}_2\text{Al}_4(\text{Al}_2\text{Si}_3\text{O}_{10})(\text{OH})_2]\)) 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.