

## **Wetting Characteristics of Oleate Monolayers Adsorbed at Calcium Mineral Surfaces: a Molecular Dynamics Study**

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*In this paper we present our Molecular Dynamics (MD) simulations results on the wettability characteristics of the surfaces of three calcium minerals namely, fluorite, calcite and fluorapatite with an adsorbed oleate monolayer in the presence of water. The contact angle of water on these oleate-adsorbed mineral surfaces are computed and compared with experimental values available in the literature. The modeled adsorbed oleate monolayers on calcite {104}, fluorite {111} and fluoroapatite {100} are packed so as to achieve the most favorable configuration, that is, 100%, 67% and 75% packing respectively.*