

DFT Theoretical Study of the Interaction of Zwitterionic Geminal Liquids with Limestone, Regarding the Behavior of the Wettability Parameter

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Zwitterionic liquids have a wide variety of applications in enhanced oil recovery. In particular, zwitterionic geminal substances have been used as wettability modifiers of limestone, dolomites and sandstones at high temperatures and pressures. The understanding of the interaction mechanisms of such molecules with the limestone surface is an important step towards the comprehension of the modification in wettability. In the study here presented, the interaction energies of limestone with zwitterionic geminal liquids of the type bis-N-alkyl polyether were calculated within the framework of the density functional theory (DFT). With the use of the CASTEP library of the Material Studio Software (a DFT-based computational code) we calculated the optimized energy density of states, and repulsion and chemisorption energies of the bis-N-alkyl polyether liquids interacting with the limestone rocks.