



سمینار هفتگی گروه ماده چگال نرم

investigation of Surfactin behavior at the presence of water, oil and asphaltene

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In this lecture, two main areas will be discussed: behavior of surfactin, as a biosurfactant, at the presence of water, oil, and asphaltene and calculation of diffusion coefficient using molecular dynamics simulation.

Enhanced Oil Recovery (EOR) is an attractive field in oil research and studies and recently, among EOR methods MEOR (Microbial Enhanced Oil Recovery) method has attracted attention of scientists. One of the most important roles in MEOR method is played by biosurfactants, produced by micro organisms. Molecular dynamics simulation of surfactin, as one of the most known biosurfactants, performed to investigate behavior of: single surfactin at water/oil interface, group of surfactins at water/oil interface, and group of surfactins at the presence of asphaltene in oil medium. Simulation results show that a single surfactin molecule can not enter into the oil phase and settles at interface, but, a group of surfactin molecules can enter into the oil phase. Furthermore, results indicate that after entering the surfactin micelles into the oil phase, they interact with asphaltene molecules by their hydrophobic tails and this hydrophobic interaction makes the surface of asphaltene aggregates hydrophilic.

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قطب ماده چگال و سیستم‌های پیچیده