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Oil Recovery and Mitigation Processes: Insights from Multiscale Molecular Simulations

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Abstract:

One of the major technological challenges in the Oil industry is to increase the oil recovery rate under an increasing regulation to reduce the environmental impact of oil production. Most of the correlated processes such as oil recovery and mitigation are based on the control interfaces and flow. In particular, with emergence of nanotechnology, this control can be at molecular level by taking advantage of processes that happens at nanoscale or by using nanostructured materials. In our group, we have explored the potentialities to go nano in order to probe the ability to displace oil: i) under confined environment at rock nanopores, ii) by controlling the chemical environment of oil/brine/rock interfaces using functionalized nanoparticles. By using an integrated multiscale computational approach ranging from first principles calculations, molecular dynamics and Lattice Boltzmann modeling, we have been able to systematically model the fluid dynamics in porous media over scales and explore the application of molecular simulations to characterize oil recovery and nanoaggregation processes under realistic oil reservoir conditions. This talk will highlight insights taken from multiscale molecular simulations to explore potential chemical additives for Enhanced Oil Recovery and investigate the effects of the interfacial and wetting properties on fluid behavior at both nano and micro scales. Also unveils the nature of nanoaggregation mechanisms of organic nanoagregates (asphaltenes) and their interactions within rock-water-oil interfaces from a much needed first principles perspective.