A sounded journey from nano to macro into everyday materials through multiscale molecular simulations

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Abstract:

Recent advances in nanostructured systems have opened a wide range of new multifunctional materials with promising potential to control interfaces and flow at nanoscale. Furthermore, the unusual physical properties of confined fluids at nanoscale can play an important role in a plethora of chemical, geochemical and environmental processes. In this talk, I will summarize some of the activities in our group at IFUSP based on multiscale molecular simulations to explore the applications of nanoscience for fluid flow through nanoporous media on everyday materials (cement, rocks, oil and water). By using an integrated bottom-up multiscale computational approach ranging from first principles calculations based on Density Functional Theory, classical molecular dynamics and Lattice Boltzmann modeling, we have been able to systematically model, characterize and investigate the effects of the interfacial and wetting properties on fluid behavior of everyday materials over scales. This approach will be illustrated with two cases: (1) water confined at cement and (2) enhanced oil recovery processes based on surface drive flow. The mobilisation of hydrocarbons trapped at the pore scale can be favored by controlling by the chemical environment through “Wetability modifiers”, such as functionalized NPs and surfactants. The methodological challenges and the potential applications in the industry will be discussed. Additionally, we have applied sonification techniques to molecular simulations, which help us to improve our perception of the phenomena at nanoscale, but also it can be used as an inspiration for music composition and enhance immersive virtual reality experiences.