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Titolo progetto : SoftNanoPores - Modeling nanoporous materials with soft interfaces

ABSTRACT

Intrusion and extrusion (IE) of liquids in nanoporous systems is important for many technological applications, such as liquid separation, liquid chromatography, energy damping/storage, porosimetry, biological/bioinspired channels, and drug delivery.

The physics of IE phenomena is based on the phase behaviour of water confined inside hydrophobic nanopores. By varying thermodynamic conditions, e.g. pressure or temperature, the stability of wet and dry pores changes, giving rise to metastabilities and transitions between the two states. Capillary theories provide a qualitative description of IE phenomena, but nowadays atomistic simulations are the tool of election for the study of IE processes. Nevertheless, current computational approaches have important limitations. The simulation of IE has been addressed so far in single pores with cylindrical geometry, which do not reflect the complexity of the interconnected pore networks in the most common mesoporous silica. Moreover, current models rely on an oversimplified description of the pore surface, which is modeled as a rigid hydrophobic surface. In practical applications, the silica surface is functionalized by flexible, organic ligands endowing it with the desired hydrophobicity. Neglecting the soft, conformationally flexible nature of the functionalizing organosilanes may hinder the observation of important physical effects affecting IE in the smallest pores.

SoftNanoPore's overcomes these limitations by developing a computationally efficient, chemically specific coarse-grained digital twin of a functionalized Si-based nanoporous materials. SoftNanoPores' digital twin will enable simulations of large porous samples with realistic geometries and interconnected pores, while explicitly accounting for the flexibility and conformational behaviour of grafting molecules on the pore surfaces.

SoftNanoPores will target the most relevant IE technologies, namely Heterogeneous Lyophobic Systems (HLS) and reverse phase High Performance Liquid Chromatography (HPLC). We will reveal the correlations between the soft hydrophobic pore interface, the geometry of the pore network and IE properties of HLS, guiding the design of efficient mechanical dampers. Furthermore, SoftNanoPores proposes an innovative approach to improve the selectivity and reduce the environmental impact of HPLC applications, based on the use of a nanofluids containing functionalized metal nanoparticles with tunable amphiphilicity.

The SoftNanopore's units have nicely complementary expertises, ranging from the development of coarse-grained models to the use of advanced sampling techniques for the characterization of IE phenomena. This, as well as the groups' international visibility and experimental collaborations, and the availability of cutting-edge high performance computing facilities, will assure the project feasibility and impact at scientific, economic, environmental and thus societal level.

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