Recently, a large effort is put to understand the variation of basic physicochemical properties of the soft matter confined at the nanoscale. Intensive studies carried out by the top research centers in the world revealed that this problem is very complex and many factors, such as the specific intermolecular interactions, wettability, interfacial energy, dynamic heterogeneities, substrate roughness, and free volume, have a strong impact on the behavior of nanosystems. In fact, among them, the roughness and density fluctuations are looming as the most important parameters controlling the molecular dynamics of glass-forming soft materials. Nevertheless, in the literature, one can find papers reporting contradictory results on the same issue. The most classical example of that is speeding or slowing down segmental dynamics in the close proximity of the rough surface. Within this project, we plan to use unique mesoporous templates characterized by nanostructured pore walls and well-defined roughness along with high-pressure impedance investigations to solve fundamental problems concerning the behavior of soft materials infiltrated into mesopores. We will focus on the verification of the existence of the irreversibly adsorbed layer in the liquids being in contact with the strongly curved nanostructured surface of the pore walls, molecular dynamics, guest-host interfacial interactions, and wettability in such systems. The other intriguing problem will be investigations of the equilibration process in pores allowing to restore bulk-like behavior in some (but not in all) examined systems upon isothermal annealing. The question is why this phenomenon happens, and what is its molecular origin? Why do some substances recover bulk dynamics, while others do not? Does this effect correlates with wettability, intermolecular interactions? Finally, we want to study the interrelationship between the dynamics of molecules adsorbed at the pore walls (interfacial layer) and the ones located closer to its center (core molecules), the kinetics of adsorption on the pore walls characterized by different morphology and roughness at ambient and elevated pressure. These unique measurements will allow us to elucidate the impact of density fluctuations on the peculiar behavior of nano soft materials.

To achieve the main goals of the project, we have selected several model low- and high-molecular-weight glass-forming liquids, which will be infiltrated into mesopores made of several materials (such us silica, alumina and zirconium dioxide) having various morphology, pore walls roughness, and diameters (d=4-150 nm). Next, we plan to perform measurements with the use of Broadband Dielectric Spectroscopy (BDS), Raman and Fourier Transform InfraRed Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM), tensiometer, etc. These experimental methods will be complemented by quantum mechanical computations (DFT) and Molecular Dynamics (MD) simulations. We are convinced that high-pressure investigations supported by multiexperimental and theoretical approaches will allow us to go much beyond the current state of the art and will contribute to a better understanding of behavior, and physicochemical properties of the systems confined at the nanoscale.