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PREFACE

Complex dynamics of fluids in disordered and crowded environments

Guest Editors

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Over the past two decades, the dynamics of fluids under nanoscale confinement has attracted much attention. Motivation for this rapidly increasing interest is based on both practical and fundamental reasons. On the practical and rather applied side, problems in a wide range of scientific topics, such as polymer and colloidal sciences, rheology, geology, or biophysics, benefit from a profound understanding of the dynamical behaviour of confined fluids. Further, effects similar to those observed in confinement are expected in fluids whose constituents have strong size or mass asymmetry, and in biological systems where crowding and obstruction phenomena in the cytosol are responsible for clear separations of time scales for macromolecular transport in the cell. In fundamental research, on the other hand, the interest focuses on the complex interplay between confinement and structural relaxation, which is responsible for the emergence of new phenomena in the dynamics of the system: in confinement, geometric constraints associated with the pore shape are imposed to the adsorbed fluids and an additional characteristic length scale, i.e. the pore size, comes into play.

For many years, the topic has been mostly experimentally driven. Indeed, a broad spectrum of systems has been investigated by sophisticated experimental techniques, while theoretical and simulation studies were rather scarce due to conceptual and computational issues. In the past few years, however, theory and simulations could largely catch up with experiments. On one side, new theories have been put forward that duly take into account the porosity, the connectivity, and the randomness of the confinement. On the other side, the ever increasing available computational power now allows investigations that were far out of reach a few years ago. Nowadays, instead of isolated state points, systematic investigations on the dynamics of confined fluids, covering a wide range of system parameters, can be realized. In fact, theory and simulations were recently able to predict new and surprising dynamical features, such as the occurrence of sub-diffusive laws, which result from the trapping due to the geometric and topological constraints and/or quenched disorder, the presence of both continuous and discontinuous glass transitions, and diffusion-localization transitions. Together, theory and simulations are thus able to contribute to a deeper insight into the complex dynamical behaviour of fluids in disordered confinement. Still, many yet unsolved problems remain.

The fact that theoretical and simulation approaches have caught up with experimental investigations, has motivated us to organize a workshop on the dynamics of fluids confined in disordered environments, so as to bring together the different communities working in this field: theory and simulations, with their recent developments based on the mode-coupling theory of the glass transition, and experiments, with particular emphasis on colloidal systems and novel techniques. In an effort to give credit to recent developments in related problems of biophysical relevance, an entire session of the programme was dedicated to anomalous diffusion in crowded environments. The workshop was thus aimed at providing a deeper understanding of the complex dynamics of fluids in confinement as well as up-to-date perspectives on the interdisciplinary applications of this field of research.

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We are proud to say that all 32 contacted speakers accepted our invitation. Additional participants were attracted by our scientific programme, contributing poster presentations to the workshop. In total, close to 50 participants were registered, arriving from 11 different countries (including the US, Japan, and Mexico). Thus we conclude that the workshop indeed addressed a highly topical scientific field. From the scientific point of view a broad range of problems was covered, ranging from biophysics over soft matter to fermion systems. From the vivid discussions it became evident that the close scientific contact between theory, simulation and experiment brought along a fruitful and mutually inspiring atmosphere. On the theoretical side, these discussions have allowed clarification of several connections between the dynamics of models of fluids in porous media (quenched-annealed, pinned particles models), those of well-known limiting cases (Lorentz gas), of realistic models of liquids with strong dynamic asymmetry (asymmetric size and mass mixtures, sodium silicates, polymers blends) and even of bulk glass-formers. On the experimental side, it appeared that soft matter systems may provide an excellent test-bed to verify the theoretical predictions. From the concluding discussion it was also clear that addressing related issues relevant to biology still remains an open challenge for the future. In view of all this, it was concluded that within a short time period a workshop with analogous scope should be organized to address the progress made on both fundamental and interdisciplinary aspects.

The realization of this workshop was made possible by generous financial support from CECAM, Centre Blaise Pascal-ENS de Lyon, and the ESF network 'Molecular Simulations in Biosystems and Material Science' (SimBioMa).