Dynamic crossover phenomena in water and other glass-forming liquids

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This special section has been inspired by the workshop on Dynamic Crossover Phenomena in Water and Other Glass-Forming Liquids, held during November 11–13, 2010 at Pensione Bencistà, Fiesole, Italy, a well-preserved 14th century Italian villa tucked high in the hills overlooking Florence. The meeting, an assembly of world renowned scientists, was organized as a special occasion to celebrate the 75th birthday of Professor Sow-Hsin Chen of MIT, a pioneer in several aspects of complex fluids and soft matter physics. The workshop covered a large variety of experimental and theoretical research topics of current interest related to dynamic crossover phenomena in water and, more generally, in other glass-forming liquids. The 30 invited speakers/lecturers and approximately 60 participants were a select group of prominent physicists and chemists from the USA, Europe, Asia and Mexico, who are actively working in the field.

Some highlights of this special section include the following works.

Professor Yamaguchi’s group and their collaborators present a neutron spin echo study of the coherent intermediate scattering function of heavy water confined in cylindrical pores of MCM-41-C10 silica material in the temperature range 190–298 K. They clearly show that a fragile-to-strong (FTS) dynamic crossover occurs at about 225 K. They attribute the FTS dynamic crossover to the formation of a tetrahedral-like structure, which is preserved in the bulk-like water confined to the central part of the cylindrical pores.

Mamontov and Kolesnikov et al study the collective excitations in an aqueous solution of lithium chloride over a temperature range of 205–270 K using neutron and x-ray Rayleigh–Brillouin (coherent) scattering. They detect both the low-frequency and the high-frequency sounds known to exist in pure bulk water above the melting temperature. They also perform neutron (incoherent) and x-ray (coherent) elastic intensity scan measurements. Clear evidence of the crossover in the dynamics of the water molecules in the solution is observed in the single-particle relaxational dynamics in the μeV (nanosecond) time scale, but not in the collective dynamics on the meV (picosecond) time scale.

Mallamace et al discuss the dynamic crossover phenomenon in both bulk water and protein hydration water. They collect previous and new experimental data from different experimental techniques and molecular dynamic simulations, and are able to develop a unified picture for the different dynamical findings.

Gallo et al present a MD study of confined water in MCM-41S-15 in order to test the applicability of Mode Coupling Theory (MCT) to the dynamics of the hydration water confined in the cylindrical pores of nominal diameter 15 Å. They find that the self dynamics of the hydration water is well described by MCT down to the crossover temperature $T_C$. However, below $T_C$ the predictions of idealized MCT no longer apply, since hopping processes intervene and water turns into a strong liquid.

Soper raises some questions as to the validity of the analysis method employed to determine the density of water confined in porous silica material MCM-41-S15 from recent neutron scattering experiments.

Professors Stanley, Franzese and his collaborators describe an efficient Monte Carlo simulation of a coarse-grained model of water to study the phase diagram of...
a water monolayer confined in a fixed disordered matrix of hydrophobic nanoparticles between two hydrophobic plates. They find a drastic change of phase behavior of the confined water, such as shortening of the liquid–liquid phase transition line, upon increasing the concentration of the hydrophobic nano-particles.

Sciortino and collaborators compute the equilibrium phase diagram of two simple models for patchy particles with three and five patches in a very broad range of pressure and temperature. The three-patch model produces a stable gas–liquid critical point.

Yun Liu et al investigate, via small angle neutron scattering and neutron spin echo measurements, the effect of temperature on dynamic cluster formation of concentrated lysozyme solutions.

Xin Li et al explore the use of the newly developed technique of spin echo small angle neutron scattering (SESANS) to investigate the structure of a colloid. They find the SESANS is able to resolve structural heterogeneity, at both intra- and inter-colloidal length scales.

The choice of the topics and their elaboration reflects both the diversified current and past research interests of Professor Chen to whom this special section of Journal of Physics: Condensed Matter is dedicated. The issue contains papers from a substantial number of the invited speakers. The papers are arranged in the three categories of water, other glass-forming liquids, and colloids.

It is our pleasure to thank all speakers, section chairs and participants who contributed to the great success of the workshop, and to all authors for their additional efforts in preparing their manuscripts. The scientific program of the workshop was organized by Professor Sow-Hsin Chen and Professor Piero Baglioni. The meeting was only possible with the generous financial support of the Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI) and the University of Florence, Italy. Finally, we express our warmest gratitude to all the members of the local organizing committee and to the staff of the CSGI for all their assistance and great efforts in organizing this meeting.