Structure and dynamics in disordered systems

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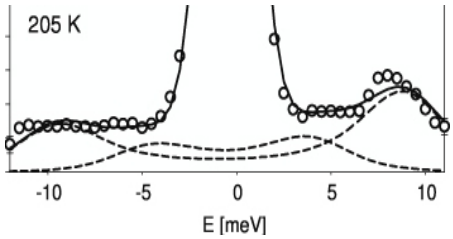
This research activity is focused on the structural and dynamical properties in disordered systems, i.e. an extremely wide class of disordered materials ranging from the broad family of liquids (simple, metallic, molecular, quantum, ionic), to glasses, including solutions, molten salts, soft (e.g. polymers) and biological matter, and aqueous systems. Our objective is to obtain a refined characterization of processes ruling the aggregation of atoms and molecules at a microscopic (anisotropic) level, because these processes are those that ultimately determine the macroscopic (isotropic) bulk and chemical-physical properties in matter.



A continuous effort is made since long time to extrapolate the properties of water in the 150-235 K range (no man's land region), where pure water unavoidably crystallizes. Here the effect of temperature on the collective modes in slightly salty water is shown.

This research addresses to both fundamental (e.g. the interaction law, polyamorphism) and technological (e.g. hydrogen storage, fuel cells, confined hydrogen in radioactive waste disposal) aspects, which may require to measure the systems properties in an extended thermodynamic range (P up to few GPa, 1 K<T 1500 K) or, other than in the bulk state, under nanometric confinement. To reach our objective we mostly use neutron and synchrotron x-ray spectroscopy, which are scattering techniques capable to cover an extended momentum-energy range (0.1- 100 nm -1 , 0.1-100 meV), thus allowing encompassing extended time- and length-scales. In particular, we have gained a longstanding experience in the experimental determination of: -structural properties (atomic and molecular correlations) by means of small- and wide-angle neutron/x-ray diffraction,, and of x-ray absorption spectroscopy; -dynamical properties such as single-particle (e.g. diffusion) and collective (e.g. sound modes) by means of quasielastic and inelastic neutron scattering techniques (three-axis and time-of-fight spectroscopy). We regularly accompany our experimental approach with intense numerical activities: -molecular simulations (classical, ab-initio) having the twofold goal of experimentally validating a model or potential, and numerically accessing a momentum-energy range even more extended than the experimental one; - the development of a Bayesian approach in the analysis of neutron scattering data, based on the exploitation of a Reversible Jump Markov Chain Montecarlo algorithm. We are especially interested in this approach as, in the case of intrinsically weak scattering data, it turns out to be extremely powerful in finding the model that better maximizes the statistical information contained in experimental data.

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