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The Dynamics of Supercooled Water

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We present an overview of recent experiments performed on transport properties of water in the deeply supercooled region, a temperature region of fundamental importance in the science of water. We report data of nuclear magnetic resonance, quasi-elastic neutron scattering, Fourier-transform infrared spectroscopy, and Raman spectroscopy, studying water confined in nano-meter-scale environments (nano-tubes and the protein hydration water) and in bulk solutions. When contained within small pores, water does not crystallise, and can be supercooled well below its homogeneous nucleation temperature Th. On this basis it is possible to carry out a careful analysis of the well known thermodynamical anomalies of water. Studying the temperature and pressure dependencies of water dynamics, we show that the liquid-liquid phase transition (LLPT) hypothesis represents a reliable model for describing liquid water. In this model, water in the liquid state is a mixture of two different local structures, characterised by different densities, namely the low density liquid (LDL) and the high-density liquid (HDL). The LLPT line should terminate at a special transition point: a low-T liquid-liquid critical point. In particular We discuss the following experimental findings on liquid water: (i) a crossover from non-Arrhenius behaviour at high T to Arrhenius behaviour at low T in transport parameters; (ii) a breakdown of the Stokes-Einstein relation; (iii) the existence of a Widom line, which is the locus of points corresponding to maximum correlation length in the p-T phase diagram and which ends in the liquid-liquid critical point; (iv) the direct observation of the LDL phase; (v) a minimum in the density at approximately 70K below the temperature of the density maximum. In our opinion these results represent the experimental proofs of the validity of the LLPT hypothesis.