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### **Supercooled aqueous solutions: a route to explore water anomalies**

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In the past years several theoretical and experimental studies have led to a picture according to which the anomalous properties of water might be due to the presence of a liquid-liquid phase transition in the supercooled region possibly terminating in a liquid-liquid critical point, LLCPC [1]. I will show molecular dynamics simulations results of ionic aqueous solutions [2,3,4] and of a solution of water and methanol [5] aimed to clarify the effect of these species on water anomalies and the LLCPC phenomenon. I will focus on the phase diagram of water in the supercooled region of the solutions in comparison with the bulk to quantify the modifications induced by the presence of the solutes. I will show that the LLCPC phenomenon persists for concentrations from low to moderate and that experimental measurements appear easier for solutions. I will also show how indications of the presence of a LLCPC nearby can come not only from thermodynamics but also from crossovers in dynamics [6,7] and from the two-body excess entropy behavior [8] as calculated from the structure [9]. I will in particular show that, similar to the bulk, the transition from a fragile behavior to a strong behavior of the liquid is present also in solutions and it is connected to the LLCPC phenomenon. These studies point out that experiments in solutions are extremely relevant for the comprehension of low temperature bulk water properties.

- [1] P. H. Poole, F. Sciortino, U. Essmann and H. E. Stanley, *Nature* 360, 324 (1992)
- [2] D. Corradini, M. Rovere and P. Gallo, *J. Chem. Phys.* 132, 134508 (2010)
- [3] D. Corradini and P. Gallo, *J. Phys. Chem. B.* 115, 14161 (2011)
- [4] P. Gallo, D. Corradini and M. Rovere, *Phys. Chem. Chem. Phys.* 13, 19814 (2011)
- [5] D. Corradini, Z. Su, H.E. Stanley and P. Gallo *J. Chem. Phys.* 137, 184503 (2012).
- [6] P. Gallo and M. Rovere, *J. Chem. Phys.* 137, 164503 (2012)
- [7] P. Gallo, D. Corradini and M. Rovere, in preparation (2013)
- [8] P. Gallo, D. Corradini and M. Rovere, *Mol. Phys.* 109, 2069 (2011)
- [9] D. Corradini, M. Rovere and P. Gallo, *J. Phys. Chem. B.* 115, 1461 (2011).