



Department Seminar:

Monday, January 22, 2018, at 11:00 a.m.;

— all are invited to meet at around 10:40 for a chat and coffee —

Prof. Lars Pettersson Theory, Chemical Physics Group,
Department of Physics,
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A Two-State Picture of Water and the Funnel of Life

PC Seminar Room G2.06, Building G, Faradayweg 4

M. Sajadi

Abstract:

I will discuss recent experimental and simulation data of liquid water and the picture of fluctuations between high-density (HDL) and low-density (LDL) liquid this has led to [1,2]. The HDL would be a more close-packed form, favored by entropy and dominates at high temperature. Below about 50°C correlated fluctuations into tetrahedral (LDL) structures, favored by hydrogen-bonding (enthalpy), begin to appear and become increasingly important upon further cooling [3,4]. A coexistence line between the two liquid phases is hypothesized, but it must lie at high pressure and low temperature in the so-called “No-man’s land” where measurements are extremely challenging due to rapid crystallization [5,6]. If such a line exists, it may terminate in a critical point from which a funnel-like region of enhanced fluctuations between the two forms emanates. Indeed, in a very recent study the isothermal compressibility and correlation length were measured down to 227 K and shown to exhibit a maximum which can be viewed as a trace of a critical point[7]. Since these fluctuations are observed up to ambient conditions we may live in what could be called the “funnel of Life”. In light of this picture I will discuss some of the more important anomalous properties of water..

[1] Anders Nilsson and Lars G.M. Pettersson, *The Structural Origin of Anomalous Properties of Liquid Water*, Nature Commun. **6**, 8998 (2015)..

[2] P. Gallo et al., *Water: A Tale of Two Liquids*, Chem. Rev. **116**, 7463-7500 (2016).

[3] L. B. Skinner et al., *The Structure of Water Around the Compressibility Minimum*, J. Chem. Phys. **141**, 214507 (2014).

[4] D. Schlesinger, K.T. Wikfeldt, L.B. Skinner, C.J. Benmore, A. Nilsson and L.G.M. Pettersson, *The temperature dependence of intermediate range oxygen-oxygen correlations in liquid water*, J. Chem. Phys. **145**, 084503 (2016).

[5] J. A. Sellberg et al., *Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature*, Nature **510**, 381 (2014).

[6] F. Perakis et al., *Diffusive dynamics during the high- to low-density transition in amorphous ices*, Proc. Natl. Acad. Sci. **114**, 8193 (2017).

[7] Kim, K.-H. et al. *Maxima in the Thermodynamic Response and Correlation Functions of Deeply Supercooled Water*, Science **358**, 1589 (2017).