

New Temperature Inversion Effect in the Thermal-Polarisation of Water

Jeff Armstrong^{C,S} and Fernando Bresme

Physical Chemistry, Imperial College London, London, United Kingdom

j.armstrong@imperial.ac.uk

Thermal coupling effects were first experimentally observed in the late 19th century by Ludwig and Soret, who famously saw the separation of binary fluids as a response to an applied temperature gradient (The Soret effect). Later experiments have exposed the complexity of the Ludwig-Soret effect. In particular it has been found that the Soret coefficient of binary mixtures can feature sign inversion. A widely studied example is represented by aqueous solutions which feature an “inversion temperature”. Above this temperature the salt is thermophobic (ions migrate towards the cold region), however below they become thermophilic^[1]. This general phenomenon is also observed in biomolecules^[2]. A full microscopic explanation of this phenomenon is still missing, although some advances have been reported recently^[3].

We have recently shown via simulation and Non-Equilibrium Thermodynamics that the permanent dipole moment of water adopts a preferred orientation by coupling to a temperature gradient, which as a result can give rise to electric fields of the order of 10^6 V/m for an applied temperature gradient of 10^1 K/ μm ^[4].

In this contribution we report the existence of an inversion temperature for the thermal polarisation of water, where the polarisation field reverses its sign. For the widely used SPC/E model we find an inversion temperature ~ 300 K at pressure ~ 400 bar. This is to best of our knowledge the first example of a temperature inversion in the thermal-polarisation of a pure liquid. Through the theory of non-equilibrium thermodynamics we provide microscopic insight into the reversal of this collective property and discuss the possibility of similar such inversion in other single component fluids.