The Thermal Polarization of Water Influences the Thermoelectric Response of Aqueous Solutions

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Thermal gradients applied to aqueous solutions give rise to fascinating coupling phenomena, such as thermophoresis (Soret) and thermoelectricity (Seebeck) effects, whereby thermal fields build concentration and charge density gradients, respectively. There is a growing interest in the understanding of the thermoelectric response of electrolyte solutions due to its relevance in a wide range of scientific and technological disciplines. Additionally, it has been highlighted that the thermoelectric effect might influence the thermophoretic response of colloids under thermal gradients [1]. The thermoelectric field appears as a consequence of the different ionic mobilities, which depend on salt concentration, composition, and charge. Thermoelectric potentials are well known in metals, and devices for energy conversion have been built using this principle. Indeed, both Soret and Seebeck effects provide a principle to design energy conversion devices. Recently, it has been shown that thermal gradients induce polarization fields in water [2]. However, the possible role of thermal orientation in determining both Seebeck and Soret effects has not been addressed systematically. Hence, more theoretical work is needed to advance our microscopic understanding of these phenomena, and to realize practical applications. We have used non-equilibrium molecular dynamics simulations to quantify the thermoelectric response of alkali halide aqueous solutions. This approach reproduces the general phenomenology of thermodiffusion in the solutions [3-4]. We examine the dependence of the Sebeeck coefficient with temperature and salt concentration and show that the thermal polarization of water plays a key role in determining the magnitude of the thermoelectric behavior of the solution.

References:

- [1] A. Würger, Phys. Rev.Lett., 101, 108302, 2008
- [2] F. Bresme et al., Phys. Rev.Lett., 101, 0031-9007, 2008.
- [3] S. Di Lecce et al., Phys. Chem. Chem. Phys, 19, 9575–9583, 2017.
- [4] S. Di Lecce et al., Sci. Rep., 7, 44833, 2017.