

Section IV

Applications of emerging materials, insulators and devices

Invited Papers

Dielectric Properties of Liquid Water: The Importance of Long-Range Interactions

Taras Bryk,^{1,2} Rodolphe Vuilleumier³ and Ari Paavo Seitsonen^{3*}

¹Institute for Condensed Matter Physics of National Academy of Sciences of Ukraine, Lviv, Ukraine

²Institute of Applied Mathematics and Fundamental Sciences, Lviv National Polytechnic University, Lviv, Ukraine

³Département de Chimie, École Normale Supérieure, Paris, France

***Email:** Ari.P.Seitsonen@iki.fi

Abstract:

The importance of the long-range, in particular the electro-static interactions, is basic knowledge in polar materials. Still many of the recent potential models, used in computer simulations of solids or liquids such as water, are based on local models of the interactions parametrised using machine learning; these kind of Machine Learning Interaction Potentials (MLIPs) have been used in several studies, providing results appearing as satisfactory.

There are recent schemes that include long-range interactions beyond the local ones. One of them is called the Latent Ewald Summation (LES) [1]. It allows the charges being fitted to the energies and forces, without needing the estimation of the atomic "charges" as input parameters to the learning.

Here we investigate the importance the inclusion of the explicit electro-static interactions, using the method LES in MLIPs, on the dielectric properties and the collective dynamics of liquid water, extending our earlier results [2] to the MLIPs, thereby enabling larger systems and longer simulations. Similar to the results reported in Ref [1] and references therein on the dipole-dipole correlations we find a qualitative error appearing at low wave numbers, or large distances in real space; furthermore we discuss the apparent short-coming in the present implementation of the LES that shows up at the very small wave numbers.

Keywords: Machine learning, Dielectric properties, Liquid water, Long-range interactions

References

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