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"Importance of van der Waals interactions in a condensed but disorder matter: Liquid water"

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London dispersion forces are due to fully non-local interaction between instantaneous dipoles. This many-body nature makes their description in density-functional theory (DFT) demanding, and in the traditionally most used for the exchange-correlation term approximations they are not present at all. The increase in the overall accuracy of DFT calculations has, however, lead to a need to include them in the calculations. Thus in the literature there have recently appeared several approaches how to treat the London dispersion forces along DFT.

Despite being the "liquid of Life" several properties of water have not been thoroughly understood. Being constituted of molecules of only three atoms and two atomic types it demonstrates a wide range of anomalies and already its frozen form, ice, exists in more than 15 different forms. This complicated phase diagram sets high requirements for the quality of description of the interactions between the atoms in water.

In this presentation we shall combine the two aspects above: First we shall review the van der Waals interactions, and describe the particolar case of water. After this we show reviews results from ab initio molecular dynamics simulations of liquid water, using different approaches to the van der Waals forces while modelling the electronic structure on-the-fly. Using modified interaction potential in classical molecular dynamics we support the conclusion of the importance of the inclusion of van der Waals forces in the simulations involving (relatively) weakly interacting molecules.

Reference:

"van der Waals effects in ab initio water at ambient and supercritical conditions", Romain Jonchiere, Ari P Seitsonen, Guillaume Ferlat, A Marco Saitta and Rodolphe Vuilleumier, Journal of Chemical Physics 135 (2011) 154503; doi:10.1063/1.3651474