Computer simulations of liquids and solvation using density functional theory-based molecular dynamics: Liquid water

A.P. Seitsonen

École Normale Supérieure, Département de Chimie, 24 rue Lhomond, F-75005 Paris, France; PSL, SU, CNRS
E–mail: Ari.P.Seitsonen@iki.fi

The computer simulation of liquids and solvation using molecular dynamics methods is a powerful tool. Its applicability depends, however, on the accuracy and the time- and length-scales of the simulations. Whereas in "classical" molecular dynamics one applies parametrised force fields to describe the interaction between the atoms, in "ab initio" molecular dynamics (AIMD) one usually relies on density functional theory (DFT) with an approximation to the exchange-correlation term chosen to reproduce satisfactorily the properties of the system under investigation. Whereas the former allows large and long-duration simulations, the latter – called DFT-based MD (DFTb-MD) by us – is better suited in simulations where there is chemical (re)activity or an accurate force field is difficult to obtain for other reasons.

We have recently applied the DFTb-MD method to the study of various properties of liquid water. In particular we have gained knowledge of the importance of the van der Waals interactions, which were not described in the most common approximations of the XC term until recent years [1,2], We also describe the simulation of the melting temperature [3] and collective dynamics of water [4].

We further discuss the extension of AIMD toward quantum chemistry methods such as MP2 and the random phase approximation (RPA).

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