Kolloquium
Theoretische Physik

Universität Konstanz

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Structural and Dynamical Properties of Liquid Water from Density Functional and Wavefunction Methods

Ab initio molecular dynamics (AIMD) has been used in the last 25 years [1] to simulate liquid water. Due to the tremendous increase in computational power and new improved algorithms great progress has been made in the understanding of basic properties of liquid water and aqueous solutions.
I will first review the history of AIMD simulations on liquids and explain the major advances in simulation techniques. Then I will give an overview on the current status of the field. For this I will mainly focus on recent developments [2] of wavefunction methods for condensed systems.

[1] K. Laasonen, M. Sprik, M. Parrinello, R. Car, JCP 99, 9080 (1993)
[2] M. Del Ben, J. Hutter, J. VandeVondele, JCP 143, 054506 (2015)