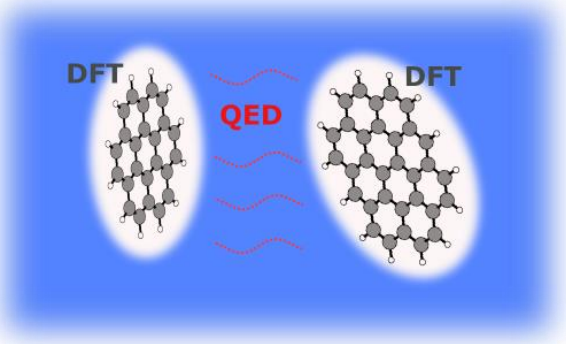
Three year DFG funded PhD position open at University of Freiburg Germany



Dispersion forces are ubiquitous in nature and result in attractive forces between atoms and molecules. A famous example is graphite, where the graphene sheets are held together solely by dispersion interactions of (vdW)–London type. The workhorse of electronic structure calculations, density functional theory (DFT), lacks sufficient dispersion interactions for most of the popular approximations. There have been successful remedies for this deficiency in order to account for dispersion forces. These improvements have so far been developed for molecules in free space only. In the context of large organic systems, the molecular constituents are typically in solution. Solvents can very efficiently be described via continuum solvent models [1]. Such an effective description of the solvent as a continuous dielectric medium does again not account for dispersion forces.

From the perspective of quantum electrodynamics (QED), London dispersion forces are the electrostatic, short-range limit of a more general quantum vacuum effect: the Casimir-Polder force. The case of objects immersed in media remains disputed. It is yet an open question how the microscopic pictures might be reconciled with the macroscopic viewpoints in a limit of large molecular systems. We will join forces from macroscopic QED and electronic structure theory in order to arrive in an effective description of van der Waals interactions in media and on surfaces.

The PhD will be located in Physics and in order to be accepted at the Institute of Physics at University of Freiburg sufficiently high marks in the master degree are needed. The PhD work will require substantial programming work, mainly in Python. Therefore experience and joy in programming are pre-conditions. Experience with electronic structure calculations and is a plus. We will develop novel approximations together with the group of S. Buhmann and will implement them to the state of the art DFT (and beyond) package GPAW and/or to the atomic simulation environment. Good communication skills in English and/or German are required.

We offer the work on a topic that bridges two so far rather separated disciplines. The University of Freiburg provides a lively research environment in a large variety of research topics. The PhD work is well funded (75% TV-L E13) for the period of three years. Last, but not least, Freiburg is a town of high living quality. Possible starting date is 1.8.2018 or as soon as possible after this date.

Please, send your application to Michael.Walter@fmf.uni-freiburg.de

http://www.functional-nanosystems.uni-freiburg.de/People/PDWalter/group

[1] A. Held, M. Walter, *J. Chem. Phys.* **2014**, *141*, 174108