Michael Walter

PD Dr.

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Scientific CV

Since 02/17	Permanent scientific employee (30%), Fraunhofer Institute for Mechanics of Materials
Since 06/15	Working group leader computational modelling, University of Freiburg, Germany
Since 02/14	Scientific employee, University of Freiburg, Germany
Since 02/13	Scientific employee, Fraunhofer Institute for Mechanics of Materials
15.12.2011	**Habilitation** in the Institute of Physics, University of Freiburg, Germany
06/08-10/13	Scientific employee, University of Freiburg, Germany
10/06-05/08	Senior postdoc, University of Jyväskylä, Finland
10/03-09/06	Postdoc, University of Jyväskylä, Finland
08/01-09/03	Scientific employee, University of Freiburg, Germany
01/01-07/01	Internet Engineer, Systor AG, Basel, Switzerland
08/00-12/00	Postdoc, University of Freiburg, Germany
21.07.2000	**Promotion** (magna cum laude) Dissertation: "Photo(doppel)ionisation von Helium und einfachen Molekülen" (Photo(double)ionization of helium and simple molecules) Supervisor: Prof. Dr. Briggs
02/97-07/00	Promotion Physik, University of Freiburg, Germany Promotion is a PhD graduation program.
09/90-01/97	Study of Physik **Diplom**, University of Freiburg, Germany Diplom 21.01.1997 ("sehr gut" = very good) Thesis: "Bestimmung der Gluondichte des Protons am ZEUS-Experiment" Supervisor: Prof. Dr. Bamberger.
07/74-05/87	School up to German Abitur

Funding

03/25-02/28	Project **Exploration of molecular mechanochromic springs: from mechanotransduction at the single chain level to stress relaxation and ageing of polymers** financed by the Deutsche Forschungsgemeinschaft (DFG), 187 k€
11/24-10/27	Project **Dual-responsive organo-sulfur network cathodes for high capacity polymer batteries** financed by DFG within SPP 2248, 174 k€
04/23-03/26	Principle investigator (PI) in the Cluster for Future **nanodiag BW** financed through the Bundesministerium für Forschung, Technologie und Raumfahrt, 144 k€.
01/19-12/25	PI in the Excellence Cluster **Living, Adaptive and Energy-autonomous Materials Systems (livMatS)** funded by the Deutsche Forschungsgemeinschaft (DFG), total Funding 36 Mio €.
11/18-10/21	Project **Force sensing and stress imaging with donor-acceptor torsional springs** funded by DFG, 136 k€
08/18-07/21	Project **HYBRIDIS: Dispersion forces in media: A hybrid approach of macroscopic quantum-wlwctrodynamics and density functional theory** funded by DFG, 136 k€
05/15-08/19	PI in the International Research Training Group (IRTG 2079) **"Cold Controlled Ensembles in Physics and Chemistry** funded by DFG, total funding 4 Mio €.
06/15-11/18	Project **Controlling the force range of polymeric force sensors made from rationally designed mechanochromic copolymer networks** funded by DFG, 130k€.
Since 2009	Computational grants on national high performance computing platforms in Karlsruhe and Jülich
10.-23.9.2006	International Wilhelm and Else Heraeus summerschool: „Few body dynamics in atomic and molecular systems" organized by Andreas Becker, Reinhard Dörner und Michael Walter

On top of these activities I have been part in several applications unofficiall, where in particular the application for a computing platform worth 260k€ has to be highlighted. My current position is connected to this positively assigned application.
Co-organized Boot-Camps and the international LivMatS conference (2023) as member of the teaching and training panel in LivMatS. Worked as scientific coordinator within the IRTG 2079 organizing summer schools in Europe and Canada.

Scientific interests

The center of my research is located in the border region between chemistry and physics, reaching out to biology and medicine. The computer based description of the electronic structure plays the central role in my studies. Topics are molecular properties, molecular interactions with and on surfaces, within functional materials and solids. Bridging of timescales that are difficult to reach by explicit simulations is achieved by the application of effective rate theories leading to insights e.g. in mechanochemistry. A long term strong interest is in modeling of spectroscopy, covering UVVis, infrared, Raman and different variants of x-ray spectroscopy.
My group benefits substantially from the density functional theory (and beyond) software GPAW as well as the atomic simulation environment ASE, and we actively participate in its development. This

allows us to extend our possibilities and to introduce new methods. In particular the advancement and refinement of spectroscopic approaches is of great interest to me. This involves the constant struggle with questions of the many body nature of matter that must be correctly taken into account in order to give a satisfying description of experimental conditions.
I have demonstrated my personal interest on the foundations of quantum mechanics by the inaugural lecture (after Habilitation) „Does God play Dice ?“.

According to google-scholar checked on Jul. 15th 2025, there are 13992 citations resulting in an H-index of 39 (https://scholar.google.com/citations?user=vlmryKEAAAAJ).

Supervision and teaching summary

My current group consists of 4 doctoral students and one masters student.

The following individuals were supervised:

PhD	Katya Zossimova (2024), Wafa Maftuhin (2023), Jan Badorrek (2022), Reyhaneh Ghassemizadeh (2019), Oliver Stauffert (2019), Rolf Würdemann (2016), Alexander Held (2015)
Master	Eleonora Galli (2024), Samaneh Khodayeki (2022), Oliver Brügner (2015)
Bachelor	Benedikt Ames (2017), Fabian Glatzel (2017), Richard Leute (2014), Thomas Reichenbach (2014), Oliver Brügner (2012)

Furthermore I have served as opponent in several PhD and Masters defenses, and reviewed several theses. I inofficially supervised the PhD-student Jens Götz, and the Maters student Ville Mäkinen.

Since my Habilitation in 2011, I give my own courses in the topics “Quantum Transport”, “Atomistic Description of Nanosystems” and “Polymer theory”. In 2015 I developed the mandatory introductory course “scientific programming” based on Python and Jupyter notebooks for the Institute of Physics at the University of Freiburg using the innovative “flipped classroom” concept. The lecture was repeated each winter semester until it was taken over by a younger colleague.

Review activities

Peer reviewed journals: J. Am. Chem. Soc., Phys. Rev. Lett., Ang. Chem. Int. Ed., Phys. Rev. A, Phys. Rev. B, Appl. Phys. Lett., Sc. Rep., J. Chem. Phys., J. Phys. Chem. Lett., J. Phys. Chem. A, Phys. Chem. Chem. Phys., Nanoscale, Particle, J. Cluster Sc., Eur. Phys. J. D, Z. Naturf., Carbon, Comp. Mat. Sc., Hybr. Mat., Int. Rev. Phys. Chem., Coord. Chem. Rev., Nanoscale
Funding agencies: Department of Energy (USA), Research Foundation Flanders (Belgium), Schweizerischer Nationalfonds (Switzerland), Deutsche Forschungsgemeinschaft (Germany), Bayerische Forschungsstiftung (Germany)

Honorary appointment

In 2014 I was elected as member of the municipal council of our village with nearly 13000 citizens.