Harald Oberhofer

Personal Details

Nationality	Austria
Birthplace	Vienna, Austria
Date of birth	20.08.1980
Affiliation	Group leader (Habilitand), Chair for Theoretical Chemistry, TU München

Education

Feb. 2008	**PhD in Physics**, *University of Vienna*, Austria, with Univ. Prof. Christoph Dellago. *(graduation with distinction)*
July 2005	**Master des Sciences de la Matière (MSc)**, *Ecole Normale Supérieure Lyon*, France.
Oct. 2004	**Diploma in Physics (MSc)**, *University of Vienna*, Austria. *(graduation with distinction)*

Work History

Feb. 2011 –	**Group leader (Habilitand)**, *Chair for Theoretical Chemistry*, Technische Universität München.
Feb. 2012 – Jan. 2014	**von Humboldt Foundation post-doctoral research fellow**, *Chair for Theoretical Chemistry*, Technische Universität München.
Feb. 2008 – Jan. 2011	**Post-Doctoral research associate**, *Department of Chemistry*, University of Cambridge.
Dec. 2004 – Jan. 2008	**Research assistant**, *Faculty of Physics*, University of Vienna.

Languages

German	mother tongue
English	fluent, spoken and written
Chinese	advanced, CEFR level B1 (2005)
French	basic, CEFR level A2 (2004)

Referee for

NSF (USA), Phys. Rev. E, J. Chem. Phys., Chem. Phys., J. R. Soc. Interface, J. Phys. Chem., J. Phys. Chem. Lett., Phys. Chem. Chem. Phys., Appl. Phys. Lett., ACS Appl. Mater. Interfaces

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Selected invited talks

2017 **"Cheap" DFT for structure prediction, and what else it is good for.**, *IMPRESS Workshop*, Helsinki, FI.

Photo-electrochemistry modelling beyond idealised surfaces and the computational hydrogen electrode , *DPG Spring Meeting*, Dresden, DE.

Photo-electrochemistry modelling beyond idealised surfaces and the computational hydrogen electrode , *GCYS Symposium on Structures & Dynamics at Surfaces*, Göttingen, DE.

2016 **First-principles photo-electrocatalysis beyond the computational hydrogen electrode**, *DPG Spring Meeting*, Regensburg, DE.

2015 **First-principles screening for intrinsic charge carrier mobility in organic devices**, *Workshop: Multiscale Simulations of Organic Electronic Materials*, Telluride, USA.

2014 **A theoretical description of water splitting on metal decorated oxide surfaces**, *9th International Conference on Functional Materials and Nanotechnologies*, Riga, Latvia.

Stability and function of organic molecular crystals, *CECAM Workshop "1st principles materials modelling"*, Lausanne, Switzerland.

2013 **Theoretical modelling of nano-structured oxide catalysts**, *TYC Seminar*, University College London, UK.

Optimisation of oxide catalysts for energy relevant processes, *CECAM Workshop "Functional Oxides"*, Bremen, Germany.

How do metal clusters split water? Towards a theoretical understanding of co-catalysts for water photo-oxidation, *Spring Meeting of the American Chemical Society*, New Orleans, USA.

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List of publications

31 **Charge Transport in Molecular Materials: an Assessment of Computational Methods**, *H. Oberhofer, K. Reuter, and J. Blumberger*, Chem. Rev. *accepted* (2017).

30 **Transferable Ionic Parameters for First-Principles Poisson-Boltzmann Solvation Calculations: Neutral Solutes in Aqueous monovalent Salt Solutions**, *S. Ringe, H. Oberhofer, and K. Reuter*, J. Chem. Phys. **146**, 134103 (2017).

29 **Consecutive reactions of small, free tantalum clusters with dioxygen controlled by relaxation dynamics**, *J.F. Eckhard, D. Neuwirth, C. Panosetti, H. Oberhofer, K. Reuter, M. Tschurl, and U. Heiz*, Phys. Chem. Chem. Phys. **19**, 5985 (2017).

28 **Perspective: On the active site model in computational catalyst screening**, *K. Reuter, C.P. Plaisance, and H. Oberhofer, M. Andersen*, J. Chem. Phys. **146**, 040901 (2017).

27 **First-Principles Free-Energy Barriers for Photoelectrochemical Surface Reactions: Proton Abstraction at TiO_2 (110)**, *T. Stecher, K. Reuter, and H. Oberhofer*, Phys. Rev. Lett. **117**, 276001 (2016).

26 **Function-Space-Based Solution Scheme for the Size-Modified Poisson-Boltzmann Equation in Full-Potential DFT**, *S. Ringe, H. Oberhofer, C. Hille, S. Matera, and K. Reuter*, J. Chem. Theor. Comput. **12**, 4052 (2016).

25 **Surface adsorption energetics studied with "Gold Standard" wave-function-based Ab initio methods: Small-molecule binding to TiO_2 (110)**, *A. Kubas, D. Berger, H. Oberhofer, D. Maganas, K. Reuter, and F. Neese*, J. Phys. Chem. Lett. **7**, 4207 (2016).

24 **Virtual Screening for High Carrier Mobility in Organic Semiconductors**, *C. Schober, K. Reuter, and H. Oberhofer*, J. Phys. Chem. Lett. **7**, 3973 (2016).

23 **Report on the sixth blind test of organic crystal structure prediction methods**, *A.M. Reilly* et al., Acta Crystallogr. Sect. B **72**, 439 (2016).

22 **Thermal and electronic fluctuations of flexible adsorbed molecules: Azobenzene on Ag (111)**, *R.J. Maurer, W. Liu, I. Poltavsky, T. Stecher, H. Oberhofer, K. Reuter, and A. Tkatchenko*, Phys. Rev. Lett. **116**, 146101 (2016).

21 **Critical analysis of fragment-orbital DFT schemes for the calculation of electronic coupling values**, *C. Schober, K. Reuter, and H. Oberhofer*, J. Chem. Phys. **144**, 054103 (2016).

20 **First-principles embedded-cluster calculations of the neutral and charged oxygen vacancy at the rutile TiO_2 (110) surface**, *D. Berger, H. Oberhofer, and K. Reuter*, Phys. Rev. B **92**, 075308 (2015).

19 **Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations II**, *A. Kubas, F. Gajdos, A. Heck, H. Oberhofer, M. Elstner, and J. Blumberger*, Phys. Chem. Chem. Phys. **17** 14342 (2015).

18 **Photoswitching in nanoporous, crystalline solids: an experimental and theoretical study for azobenzene linkers incorporated in MOFs**, *Z. Wang, L. Heinke, J. Jelic, M. Cakici, M. Dommaschk, R. J. Maurer, H. Oberhofer, S. Grosjean, R. Herges, S. Bräse, K. Reuter, and C. Wöll*, Phys. Chem. Chem. Phys. **17**, 14582 (2015).

17 **Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework**, *D. Berger, A.J. Logsdail, H. Oberhofer, M.R. Farrow, C.R.A. Catlow, P. Sherwood, A.A. Sokol, V. Blum, and K. Reuter*, J. Chem. Phys. **141**, 24105 (2014).

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16 **Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations**, *A. Kubas, F. Hoffmann, A. Heck, H. Oberhofer, M. Elstner, J. Blumberger*, J. Chem. Phys. **140**, 104105 (2014).

15 **Chemical activity of thin oxide layers: Strong support interactions yielding a new thin film phase of ZnO**, *V. Schott, H. Oberhofer, A. Birkner, M. Xu, Y. Wang, K. Reuter, and Ch. Wöll*, Ang. Chem. Int. Ed. **52**, 11925 (2013).

14 **First-principles thermodynamic screening approach to photo-catalytic water splitting with co-catalysts**, *H. Oberhofer and K. Reuter*, J. Chem. Phys. **139**, 044710 (2013).

13 **On the inapplicability of electron-hopping models for the organic semiconductor phenyl-C_{61}-butyric acid methyl ester (PCBM)**, *F. Gajdos, H. Oberhofer, M. Dupuis, and J. Blumberger*, J. Phys. Chem. Lett. **4**, 1012 (2013).

12 **Revisiting electronic couplings and hopping models for electron transport in crystalline C_{60} at ambient temperatures**, *H. Oberhofer and J. Blumberger*, Phys. Chem. Chem. Phys. **14**, 13846 (2012).

11 **Proton transfer drives protein radical formation in Helicobacter pylori catalase but not in Penicillium vitale catalase**, *M. Alfonso-Prieto, H. Oberhofer, M.L. Klein, C. Rovira, and J. Blumberger*, J. Am. Chem. Soc. **133**, 4285 (2011).

10 **Insight into the mechanism of the Ru^{2+} - Ru^{3+} electron self-exchange reaction from quantitative rate calculations**, *H. Oberhofer and J. Blumberger*, Ang. Chem. Int. Ed. **49**, 3631 (2010).

9 **Electronic coupling matrix elements from charge constrained density functional theory calculations using a plane wave basis set**, *H. Oberhofer and J. Blumberger*, J. Chem. Phys. **133**, 4103 (2010).

8 **Prediction of Reorganization Free Energies for Biological Electron Transfer: A Comparative Study of Ru-Modified Cytochromes and a 4-Helix Bundle Protein**, *V. Tipmanee, H. Oberhofer, M. Park, K.S. Kim, and J. Blumberger*, J. Am. Chem. Soc. **132**, 17032 (2010).

7 **Efficient extraction of free energy profiles from non-equilibrium experiments**, *H. Oberhofer and C. Dellago*, J. Comp. Chem. **30** 1726 (2009).

6 **Charge constrained density functional molecular dynamics for simulation of condensed phase electron transfer reactions**, *H. Oberhofer and J. Blumberger*, J. Chem. Phys. **131**, 064101 (2009).

5 **Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes**, *M. Marksteiner, P. Haslinger, H. Ulbricht, M. Sclafani, H. Oberhofer, C. Dellago, and M. Arndt*, J. Am. Soc. Mass. Spectr. **19**, 1021 (2008).

4 **Optimum bias for fast-switching free energy calculations**, *H. Oberhofer and C. Dellago*, Comp. Phys. Commun. **179**, 41 (2008).

3 **Single molecule pulling with large time steps**, *H. Oberhofer, C. Dellago, and S. Boresch*, Phys. Rev. E **75**, 061106 (2007).

2 **Equilibrium free energies from fast-switching trajectories with large time steps**, *W. Lechner, H. Oberhofer, C. Dellago, P.L. Geissler*, J. Chem. Phys. **124**, 044113 (2006).

1 **Biased sampling of nonequilibrium trajectories: Can fast switching simulations outperform conventional free energy calculation methods?**, *H. Oberhofer, C. Dellago, and P. L. Geissler*, J. Phys. Chem. B **109**, 6902 (2005).

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Teaching

2017 **Lecture: "Molecular Structure and Statistical Thermodynamics"**, *TU Munich, Germany*.
(Undergraduate level)

2014–2017 **Lecture: "Introduction to Quantum Mechanics"**, *TU Munich, Germany*.
(Undergraduate level)

2014–2016 **Lecture: "Solid State Theory"**, *TU Munich, Germany*.
(Master level)

2012–2014 **Lecture: "Advanced Electronic Structure "**, *TU Munich, Germany*.
(Master level)

2012–2014 **Lecture: "Methods of Molecular Simulation"**, *TU Munich, Germany*.
(Master level)

2011 **Lecture: "Current Topics in Theoretical Chemistry"**, *TU Munich, Germany*.
(Master level)

2008–2010 **Supervisions: "Electronic Structure", "Perturbation Theory", "Theoretical techniques and ideas in Chemistry", "Energetics and Equilibria", "Chemical Kinetics", "Quantum Mechanics", and "Spectroscopy"**, *various colleges, Cambridge, UK*.
(Undergraduate level)

Fellowships and grants

2016 **DFG Research Grant**, *"Theoretical Investigation of Photo-Electro-Catalysis Beyond Proton-Coupled Electron Transfer"*, (Volume: 1 PhD position, 3 years; travel money).

2016 **DFG Focus Program SPP 1928**, *"Development of Electrically Conductive MOFs and their Integration in Multiparametric MOF@SAW Sensor Devices"*, (Volume: 1 PhD position, 3 years; travel money).

2015 – **PI in "Solar Technologies go Hybrid" program of the state of Bavaria**.

2012 – 2014 **von Humboldt Foundation post-doctoral research fellowship**.

2013 **BayIntAn travel grant for the initiation of international collaborations**.

2011 **SuperMUC computing grant**, *together with Prof. K. Reuter*, (Volume: 4 mil. Core hours).

2010 **PRACE early access computing grant**, *together with Dr. J. Blumberger*, (Volume: 25 mil. Core hours).

(Oct. 2009 - April 2011) **College research associateship**, *Clare College, Cambridge*.

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