

## **Prof. Dr. Karsten Reuter**

Fritz-Haber-Institut der Max-Planck-Gesellschaft  
Abteilung Theorie, Faradayweg 4-6, 14195 Berlin and  
+49 30 8413 4700, reuter@fhi-berlin.mpg.de

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### **Education**

Habilitation	Theoretical Physics, FU Berlin, Germany, 2005
Ph.D.	Theoretical Physics, Universität Erlangen-Nürnberg, Germany / Universidad Autónoma de Madrid, Spain, 1998
Diplom	Physics, Universität Erlangen-Nürnberg, Germany, 1995

### **Experience**

Director, Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, 2020-present

Chair for Theoretical Chemistry & Catalysis Research Center,  
Technische Universität München, Germany  
Full Professor in Chemistry, Adjunct Professor in Physics, 2009-2020

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany  
Head of MPG Independent Junior Research Group “First-Principles Statistical Mechanics”, 2005-2009

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany  
Group Leader “Catalytic Reactions at Surfaces”, Theory Department, 2003-2005

FOM Instituut voor Atom- en Molecuulfysica AMOLF, Amsterdam, The Netherlands  
DFG Fellow, 2002-2003

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany  
Research Associate, Theory Department, 1999-2002



### **Fellowships, Awards and Professional Recognition (selection)**

Visiting Professor, Dept. of Materials, Imperial College London, 2019-2020  
Lectureship of the Netherlands Center for Multiscale Catalytic Energy Conversion, 2019  
Visiting Professor, Dept. of Mechanical Engineering, MIT, U.S.A., 2018  
MPG Frontiers Award for Chemical Energy Conversion, 2018  
Visiting Professor, Dept. of Chemical Engineering, Stanford University, U.S.A., 2014-2015  
MPG Independent Junior Group Award, 2005  
German Research Foundation (DFG) Fellowship, 2002

### **Commissions of Trust and Memberships (only current)**

Chair, Division of Surface Science, German Physical Society DPG, 2020-present  
Spokesperson, DFG Cluster of Excellence *e*-conversion, 2019-present  
Member, Int. Advisory Board, Journal of Molecular Modeling, Springer, 2018-present  
Member, Executive Board, Leibniz Supercomputing Center, Munich, 2016-present  
Member, Executive Committee, Research Consortium Solar Technologies Go Hybrid, 2014-present  
Member, Scientific Committee, Symposium on Surface Science, 2014-present  
Member, Int. Advisory Board, Advanced Materials Interfaces, Wiley, 2013-present  
Member and Work Package Leader, Int. Advisory Board, Psi-k Network, 2009-present  
Chair, Int. Advisory Board, European Conference on Surface Crystallography and Dynamics, 2007 –

## **Scientific Interests**

Predictive-quality multiscale materials modeling  
Data analytics and machine learning  
Energy conversion at interfaces, including heat dissipation  
Heterogeneous oxidation catalysis and electrocatalysis, including oxide formation and corrosion  
(Photo-)electrochemistry and organic solar cells  
Surface nanotechnology, including molecular electronics, adsorption dynamics and self-assembly  
Novel (catalytic and energy) materials, especially framework materials and solid-state electrolytes

## **Selected Recent Publications (Total: 237, WoS h-Index 55, Google Scholar 64)**

1. A. Bruix, J.T. Margraf, M. Andersen, K. Reuter, *First-Principles Based Multiscale Modeling of Heterogeneous Catalysis*, *Nature Catal.* **2**, 659 (2019).
2. D. Opalka, C. Scheurer, K. Reuter, *Ab Initio Thermodynamics Insight into the Structural Evolution of Working IrO<sub>2</sub> Catalysts in Proton-Exchange Membrane Electrolyzers*, *ACS Catal.* **9**, 4944 (2019).
3. M. Andersen, S.V. Levchenko, M. Scheffler, K. Reuter, *Beyond Scaling Relations for the Description of Catalytic Materials*, *ACS Catal.* **9**, 2752 (2019).
4. H.H. Heenen, C. Scheurer, K. Reuter, *Implications of Occupational Disorder on Ion Mobility in Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> Battery Materials*, *Nano Lett.* **17**, 3884 (2017).
5. C. Schober, K. Reuter, H. Oberhofer, *Virtual Screening for High Carrier Mobility in Organic Semiconductors*, *J. Phys. Chem. Lett.* **7**, 3973 (2016).
6. M. Andersen, A.J. Medford, J.K. Nørskov, K. Reuter, *Analyzing the Case for Bifunctional Catalysis*, *Angew. Chemie Int. Ed.* **55**, 5210 (2016).
7. T. Stecher, K. Reuter, H. Oberhofer, *First-Principles Free-Energy Barriers for Photo-Electrochemical Surface Reactions: Proton Abstraction at TiO<sub>2</sub>(110)*, *Phys. Rev. Lett.* **117**, 276001 (2016).
8. A.C. Luntz, J. Voss, K. Reuter, *Interfacial Challenges in Solid-State Li Ion Batteries*, *J. Phys. Chem. Lett.* **6**, 4599 (2015).
9. J. Meyer, K. Reuter, *Modeling Heat Dissipation at the Nanoscale: An Embedding Approach for Chemical Reaction Dynamics on Metal Surfaces*, *Angew. Chemie Int. Ed.* **53**, 4721 (2014).
10. S. Matera, M. Maestri, A. Cuoci, K. Reuter, *Predictive-Quality Surface Reaction Chemistry in Real Reactor Models: Integrating First-Principles Kinetic Monte Carlo Simulations Into Computational Fluid Dynamics*, *ACS Catal.* **4**, 4081 (2014).

## **Organization of Scientific Meetings (selection)**

Annual Int. Workshop on Frontiers of Multiscale Modeling in Materials, Energy & Catalysis, 2014 –2020  
Multiple CECAM and Psi-k Workshops and Schools, e.g. Electronic Structure Theory with Numeric Atomic Orbitals, or Catalysis from First Principles (Cat1p), 2003 – 2019  
Co-Chair, European Conference on Surface Science (ECOSS-29), together with CMD-24, CMMP-12 and ECSCD-11 (> 1.000 participants), 2012  
Co-Organizer, IPAM Workshop on Bridging Time and Length Scales in Materials Science and Bio-Physics, 3-month program at Institute for Pure and Applied Mathematics (IPAM), UCLA, USA, 2005

## **Research Supervision**

In the last 15 years, 26 students received a PhD under his direct supervision; currently he is supervising 19 PhD students. 45 postdocs have worked in his group during the last 15 years, including 10 researchers at present. 18 were financed by an Alexander von Humboldt fellowship. For his particular involvement with Chinese students, he received the 2016 “Best Student Supervisor Award” from the German Society of Chinese Chemists and Chemical Engineers.

## **Post Doctoral and Thesis Advisors**

Klaus Heinz, Institut für Festkörperphysik, Universität Erlangen-Nürnberg, Germany  
Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany  
Daan Frenkel, FOM Inst. AMOLF, Amsterdam, The Netherlands (now Cambridge University, UK)