

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

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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



### **Academic Positions**

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

Distinguished Affiliated Professor,  
Technische Universität München, Germany, 2021-present

Honorary Professor, Chemistry,  
Humboldt Universität zu Berlin, Germany, 2021-present

Honorary Professor, Physics,  
Free University Berlin, Germany, 2021-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

### **Scientific Interests**

Predictive-quality multiscale modeling  
Data analytics and machine learning  
Energy conversion at interfaces, including heat dissipation  
Heterogeneous catalysis (thermal and electro), operando evolution incl. oxide formation and corrosion  
Surface nanotechnology, including molecular electronics, adsorption dynamics and self-assembly  
Novel (catalytic and energy) materials, especially framework materials and solid-state electrolytes

### **Visiting Appointments, Awards and Professional Recognition (selection)**

Elected Henriette-Herz Scout, Alexander von Humboldt Society, 2021-present  
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

### **Active Leadership Roles (selection)**

Member, Supervisory Board, Helmholtz Center Berlin, 2022-present  
PI, DFG Cluster of Excellence Unisyscat, 2021-present  
Chair, Division of Surface Science, German Physical Society DPG, 2020-present  
Spokesperson, DFG Cluster of Excellence *e*-conversion, 2019-present  
Member, Int. Advisory Board, Max Planck Computing and Data Facility, 2019-present  
Member, Int. Advisory Board, Journal of Molecular Modeling, Springer, 2018-present  
Member, Scientific Committee, Symposium on Surface Science, 2014-present  
Member and Work Package Leader, Int. Advisory Board, Psi-k Network, 2009-present  
Chair, Int. Advisory Board, Europ. Conference on Surface Crystallography and Dynamics, 2007-present

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

Annual Int. Workshop on Frontiers of Multiscale Modeling in Materials, Energy & Catalysis, 2014 –2021  
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, 29 students received a PhD under his direct supervision; currently he is supervising 32 PhD students. 56 postdocs and scientific staff have worked in his group, including 23 researchers at present. 15 received an Alexander von Humboldt fellowship, and 19 alumni have by now secured tenured faculty positions in academia. 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.

### **Conference Presentations**

>230 invited and plenary talks, >110 departmental seminars. Recent selected keynotes and plenaries: 72<sup>nd</sup> Annual Meeting of the Int. Society of Electrochemistry, online (2021); Electronic Materials and Applications EMA2021, online (2021); Condensed Matter Conference CMD2020, online (2020); 34<sup>th</sup> DECHEMA Jahrestagung, online (2020); 47<sup>th</sup> Congress of the Int. Union of Pure and Applied Chemistry, Paris (2019); 66<sup>th</sup> Symposium of the American Vacuum Society, Columbus (2019); VI San Luis Conference on Surfaces, Interfaces and Catalysis, Santa Fe (2018); 11<sup>th</sup> Congress on Electronic Structure: Principles and Applications, Toledo (2018).

## **Recent Representative Publications (Total: 283, WoS h-Index 64, Google Scholar 74)**

1. C. Kunkel, J.T. Margraf, K. Chen, H. Oberhofer, and K. Reuter, *Active Discovery of Organic Semiconductors*, Nature Commun. **12**, 2422 (2021).
2. J.T. Margraf and K. Reuter, *Pure, Non-local, Machine-Learned Density Functional Theory for Electron Correlation*, Nature Commun. **12**, 344 (2021).
3. S. Stocker, G. Csányi, K. Reuter, J.T. Margraf, *Machine Learning in Chemical Reaction Space*, Nature Commun. **11**, 5505 (2020).
4. A. Bruix, J.T. Margraf, M. Andersen, K. Reuter, *First-Principles Based Multiscale Modeling of Heterogeneous Catalysis*, Nature Catal. **2**, 659 (2019).
5. 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).
6. M. Andersen, S.V. Levchenko, M. Scheffler, K. Reuter, *Beyond Scaling Relations for the Description of Catalytic Materials*, ACS Catal. **9**, 2752 (2019).
7. 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).
8. K. Reuter, *Ab Initio Thermodynamics and First-Principles Microkinetics for Surface Catalysis*, Catal. Lett. **146**, 541 (2016).
9. C. Schober, K. Reuter, H. Oberhofer, *Virtual Screening for High Carrier Mobility in Organic Semiconductors*, J. Phys. Chem. Lett. **7**, 3973 (2016).
10. A.C. Luntz, J. Voss, K. Reuter, *Interfacial Challenges in Solid-State Li Ion Batteries*, J. Phys. Chem. Lett. **6**, 4599 (2015).