Prof. Dr. Karsten Reuter

Fritz-Haber-Institut der Max-Planck-Gesellschaft
Theory Department, Faradayweg 4-6, 14195 Berlin, Germany
+49 30 8413 4700, reuter@fhi-berlin.mpg.de, https://www.fhi.mpg.de/th-department

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

Scientific Director,
BasCat Unicat-BASF Joint Lab, Berlin, Germany, 2023-present

Distinguished Affiliated Professor, Technische Universität München, Germany, 2023-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 and charge transport
Heterogeneous catalysis (thermal and electro), operando evolution incl. oxide formation and corrosion
Novel (catalytic and energy) materials, especially solid-state electrolytes and solar battery materials
Surface nanotechnology, including molecular electronics, adsorption dynamics and self-assembly

Visiting Appointments, Awards and Professional Recognition (selection)

Visiting Fellow, Pembroke College, University of Cambridge, UK, 2025-present
Fellow, European Laboratory for Learning and Intelligent Systems (ELLIS), 2023-present
Elected Henriette-Herz Scout, Alexander von Humboldt Society, 2021-present
Visiting Professor, Dept. of Materials, Imperial College London, UK, 2019-2020
Lectureship of the Netherlands Center for Multiscale Catalytic Energy Conversion, 2019
Visiting Professor, Dept. of Mechanical Engineering, MIT, USA, 2018
MPG Frontiers Award for Chemical Energy Conversion, 2018
Visiting Professor, Dept. of Chemical Engineering, Stanford University, USA, 2014-2015
MPG Independent Junior Group Award, 2005

Active Leadership Roles (selection)

Member, Council, German Physical Society DPG, 2024-present
Member, Scientific Advisory Board, Federal Institute for Materials Research and Testing, 2023-present
PI and Area Coordinator, DFG Cluster of Excellence e-conversion, 2023-present
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, 2020-2022
Spokesperson, DFG Cluster of Excellence e-conversion, 2019-2023
Member, Int. Advisory Board, Max Planck Computing and Data Facility, 2019-present
Member, Scientific Committee, Symposium on Surface Science, 2014-present
Trustee and Member of Int. Advisory Board, Psi-k Network, 2009-present
Chair, Int. Advisory Board, Europ. Conference on Surface Crystallography and Dynamics, 2007-present
Member of various Editorial Advisory Boards (Adv. Intelligent Systems, J. Chem. Phys., …)

Organization of Scientific Meetings (selection)

Annual Int. Workshop on Frontiers of Multiscale Modeling in Materials, Energy & Catalysis, 2014 –2025
Numerous CECAM and Psi-k Workshops and Schools, e.g. Electronic Structure Theory with Numeric Atomic Orbitals, or Catalysis from First Principles (Cat1p), 2003 – 2025
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 20 years, 46 students received a PhD under his direct supervision; currently he is supervising 32 PhD students. 79 postdocs and scientific staff have worked in his group, including 31 researchers at present. 24 received an Alexander von Humboldt fellowship, and 27 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

>280 invited, keynote and plenary talks, >120 departmental seminars. Recent selected keynotes and plenaries: Annual Meeting of the German Catalysis Society, Weimar (2025); Comp. Molecular Science, Warwick (2024); Int. Conf. on Data-Integrated Simulation Science, Stuttgart (2023); 28th North American Catalysis Society Meeting, Providence (2023); 22nd International Vacuum Congress, Sapporo (2022), 73rd Annual Meeting of the Int. Society of Electrochemistry, online (2022); Electronic Materials and Applications EMA2021, online (2021).

Recent Representative Publications (Total: 339, Google Scholar h-index: 89)

1. K.C. Lai, P. Poths, S. Matera, C. Scheurer, and K. Reuter, *Automatic Process Exploration through Machine-Learning Assisted Transition State Searches*, Phys. Rev. Lett. **134**, 096201 (2025).

2. C. Scheurer and K. Reuter, *Role of the Human-in-the-Loop in Emerging Self-Driving Laboratories for Heterogeneous Catalysis*, Nature Catal. **8**, 13 (2025).

3. H.H. Heenen, H.S. Pillai, K. Reuter, and V.J. Bukas, *Exploring Mesoscopic Mass Transport Effects on Electrocatalytic Selectivity*, Nature Catal. **7**, 847 (2024).

4. J.T. Margraf, H. Jung, C. Scheurer, and K. Reuter, *Exploring Catalytic Reaction Networks with Machine Learning*, Nature Catal. **6**, 112 (2023).

5. S. Ringe, N.G. Hörmann, H. Oberhofer, and K. Reuter, *Implicit Solvation Methods for Catalysis at Electrified Interfaces*, Chem. Rev. **122**, 10777 (2022).

6. S.D. Beinlich, N.G. Hörmann, and K. Reuter, *Field Effects at Protruding Defect Sites in Electrocatalysis at Metal Electrodes?*, ACS Catal. **12**, 6143 (2022).

7. C. Kunkel, J.T. Margraf, K. Chen, H. Oberhofer, and K. Reuter, *Active Discovery of Organic Semiconductors*, Nature Commun. **12**, 2422 (2021).

8. J.T. Margraf and K. Reuter, *Pure, Non-local, Machine-Learned Density Functional Theory for Electron Correlation*, Nature Commun. **12**, 344 (2021).

9. S. Stocker, G. Csányi, K. Reuter, J.T. Margraf, *Machine Learning in Chemical Reaction Space*, Nature Commun. **11**, 5505 (2020).

10. A. Bruix, J.T. Margraf, M. Andersen, K. Reuter, *First-Principles Based Multiscale Modeling of Heterogeneous Catalysis*, Nature Catal. **2**, 659 (2019).