

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.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, machine learning and artificial intelligence (AI)
Energy conversion at interfaces, including heat dissipation and charge transport
Heterogeneous catalysis (thermal and electro), operando evolution incl. degradation and rejuvenation
AI for experiment planning and control, self-driving laboratories
Novel (catalytic and energy) materials, especially solid-state electrolytes and solar battery materials
Surface nanotechnology, including molecular electronics, surface dynamics and self-assembly

Visiting Appointments, Awards and Professional Recognition (selection)

Honorary Fellow, Chinese Chemical Society, 2026-present
ERC Synergy Grant, 2025-present
Guest Professor, Hokkaido University, J, 2025-present
Visiting Fellow, Pembroke College, University of Cambridge, UK, 2025-2026
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, Scientific Advisory Board, Dunia Innovations, GmbH, 2026-present
Member, Scientific Council, African Network ASESMANET, 2026-present
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
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 –2026
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

Research Supervision

In the last 20 years, 48 students received a PhD under his direct supervision; currently he is supervising 36 PhD students. 85 postdocs and scientific staff have worked in his group, including 30 researchers at present. 25 received an Alexander von Humboldt fellowship, and 30 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 Chin. Chemists and Chemical Engineers.

Conference Presentations

>290 invited, keynote and plenary talks, >120 departmental seminars. Recent selected keynotes and plenaries: AI4X – Accelerated Conf., Singapore (2026); 18th Int. Congr. of Quantum Chemistry, Berkeley (2026); 26th Asian Conf. on Electronic Structure Theory, Tsukuba (2025); 38th Eur. Conf. on Surface Science, Braga (2025), Ann. Meeting of the German Catalysis Society, Weimar (2025).

Recent Representative Publications (Total: 371, Google Scholar h-index: 95)

1. K.S. Jakob, A. Walsh, K. Reuter, and J.T. Margraf, *Learning Crystallographic Disorder: Bridging Prediction and Experiment in Materials Discovery*, Adv. Mater. **38**, e14226 (2026).
2. F. Riccius, N. Bergmann, H.H. Heenen, and K. Reuter, *Out of the Crystalline Comfort Zone: Sampling the Initial Oxide Formation at Cu(111)*, Adv. Sci. **12**, e13878 (2025).
3. N. Bergmann, N. Bonnet, N. Marzari, K. Reuter, and N.G. Hörmann, *Machine Learning the Energetics of Electrified Solid/Liquid Interfaces*, Phys. Rev. Lett. **135**, 146201 (2025).
4. 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).
5. 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).
6. 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).
7. W. Xu, E. Diesen, T. He, K. Reuter, and J.T. Margraf, *Discovering High Entropy Alloy Electrocatalysts in Vast Composition Spaces with Multi-Objective Optimization*, J. Am. Chem. Soc. **146**, 7698 (2024).
8. J.T. Margraf, H. Jung, C. Scheurer, and K. Reuter, *Exploring Catalytic Reaction Networks with Machine Learning*, Nature Catal. **6**, 112 (2023).
9. S. Ringe, N.G. Hörmann, H. Oberhofer, and K. Reuter, *Implicit Solvation Methods for Catalysis at Electrified Interfaces*, Chem. Rev. **122**, 10777 (2022).
10. A. Bruix, J.T. Margraf, M. Andersen, K. Reuter, *First-Principles Based Multiscale Modeling of Heterogeneous Catalysis*, Nature Catal. **2**, 659 (2019).