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

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)

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, 26 students received a PhD under his direct supervision; currently he is supervising 30 PhD students. 51 postdocs and scientific staff have worked in his group, including 18 researchers at present. 14 received an Alexander von Humboldt fellowship, and 17 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

>220 invited and plenary talks, >110 departmental seminars. Recent selected keynotes and plenaries: 72nd Annual Meeting of the Int. Society of Electrochemistry, online (2021); Electronic Materials and Applications EMA2021, online (2021); Condensed Matter Conference CMD2020, online (2020); 34th DECHEMA Jahrestagung, online (2020); 47th Congress of the Int. Union of Pure and Applied Chemistry, Paris (2019); 66th Symposium of the American Vacuum Society, Columbus (2019); VI San Luis Conference on Surfaces, Interfaces and Catalysis, Santa Fe (2018); 11th Congress on Electronic Structure: Principles and Applications, Toledo (2018).

Recent Representative Publications (Total: 264, WoS h-Index 62, Google Scholar 72)

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_2 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 $Li_4Ti_5O_{12}$ 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).