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

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, 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, 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: 246, WoS h-Index 57, Google Scholar 66)

1. S. Stocker, G. Csányi, K. Reuter, J.T. Margraf, *Machine Learning in Chemical Reaction Space*, Nature Commun. **11**, 5505 (2020).
2. A. Bruix, J.T. Margraf, M. Andersen, K. Reuter, *First-Principles Based Multiscale Modeling of Heterogeneous Catalysis*, Nature Catal. **2**, 659 (2019).
3. 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).
4. M. Andersen, S.V. Levchenko, M. Scheffler, K. Reuter, *Beyond Scaling Relations for the Description of Catalytic Materials*, ACS Catal. **9**, 2752 (2019).
5. 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).
6. K. Reuter, *Ab Initio Thermodynamics and First-Principles Microkinetics for Surface Catalysis*, Catal. Lett. 146, 541 (2016).
7. C. Schober, K. Reuter, H. Oberhofer, *Virtual Screening for High Carrier Mobility in Organic Semiconductors*, J. Phys. Chem. Lett. **7**, 3973 (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 Math-ematics (IPAM), UCLA, USA, 2005

Research Supervision

In the last 15 years, 26 students received a PhD under his direct supervision; currently he is supervising 23 PhD students. 48 postdocs have worked in his group during the last 15 years, including 13 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)