

Curriculum Vitae Prof. Dr. Axel Groß, April 2025

PERSONAL INFORMATION

Groß, Axel

Researcher unique identifier: Research ID B-4023-2014, ORCID ID: 0000-0003-4037-7331

Nationality: German

Date of birth: 30.12.1961

URL of homepage: <http://www.uni-ulm.de/theochem>

EDUCATION

- 1999 Habilitation in Theoretical Physics, Technical University of Berlin, title of habilitation thesis *Reactions at surfaces studied by ab initio dynamics calculations*
- 1993 Ph.D. Physics Department, Technical University of Munich, title of Ph.D. thesis *Vibrational excitation of diatomic molecules in the scattering from surfaces*
- 1990 Diploma of Physics, University of Göttingen, title of diploma thesis *Real-space formalism for total energy calculations of semiconductors*

CURRENT POSITIONS

- 2011 - PI at the Helmholtz Institute Ulm – Electrochemical Energy Storage
- 2004 - Full Professor and Director of the Institute of Theoretical Chemistry, Ulm University

PREVIOUS POSITIONS

- 1998 - 2004 Associate Professor for Theoretical Physics/Surface Physics, Physics Department, Technical University of Munich
- 1993 - 1998 Staff scientist, Department of Theory, Fritz-Haber-Institute, Berlin
- 1990 - 1993 Research assistant, Physics Department, Technical University of Munich

STAYS ABROAD

- 2014 Visiting professor (Prof. Jens Nørskov), Department of Chemical Engineering, Stanford University, CA, USA (2 months)
- 2005 Visiting professor (Prof. Horia Metiu), Chemistry Department of the University of California at Santa Barbara, USA (1 month)
- 1996 Visiting scientist (Prof. D. Papaconstantopoulos) at the Naval Research Lab, Washington, D.C., USA, Complex Systems Theory Branch (1 1/2 months)
- 1986 - 1987 Exchange student, University of California at Santa Barbara, USA (1 year)

FELLOWSHIPS AND AWARDS

- 2007 - 2013 Three PhD awards for students supervised by the PI
- 2002 Lecturing award, Technical University of Munich
- 1986 Fulbright travel grant

SUPERVISION OF GRADUATE STUDENTS

- 1996- Supervision of 23 Master students, 27 PhD students and 22 PostDocs at the Fritz-Haber-Institute, Berlin, the Technical University of Munich, and Ulm University

TEACHING ACTIVITIES

- 1998- Regular teaching activities according to the requirements for German professors (nine hours per week) in Theoretical Physics at the Technical University of Munich and in Theoretical Chemistry at Ulm University

ORGANISATION OF SCIENTIFIC MEETINGS

- 1999- (Co-)Organization of 20 international workshops, conferences and symposia, four recent ones are given below
- Oct 22-26, 2022 Workshop “Computational modelling of batteries: First-principles quantum chemistry meets continuum approaches”, Castle Reisenburg near Ulm
- Jul 28-Aug 2, 2019 Gordon Research Conference on “Dynamics at Surfaces”, Newport, RI, US
- Nov. 26-29, 2017 Workshop “The electrode potential in electrochemistry – A challenge for electronic structure theory calculations”, Castle Reisenburg near Ulm

INSTITUTIONAL RESPONSIBILITIES

- 2021 - Member of the Managing Board of the AG Theoretical Chemistry
- 2019 - Spokesperson of the Cluster of Excellence EXC 2154 “Energy storage beyond Lithium” of the German Science Foundation
- 2012 - 2015 Vice-President for Research of Ulm University
- 2010 - 2016 Spokesperson of the Research Unit FOR 1376 of the German Science Foundation “Elementary reaction steps in electrocatalysis: Theory meets experiment”
- 2012 - 2014 Spokesperson of the Surface Science Section of the German Physical Society
- 2010 - 2012 Vice-Spokesperson of the Surface Science Section of the German Physical Society
- 2009 - 2012 Dean of the Faculty of Natural Sciences, Ulm University
- 2008 - 2009 Study Dean of the Department of Chemistry, Ulm University
- 2006 - 2008 Vice-Dean of the Faculty of Natural Sciences, Ulm University

COMMISSIONS OF TRUST

- 2020-2024 Re-elected Member of the Review Board of the German Science Foundation
- 2016-2020 Elected Member of the Review Board of the German Science Foundation
- 2018 - Member of the Board of Trustees of the Dr. Barbara Mez-Starck Foundation
- 2018 Member of the Evaluation Board of DTU Physics, Lyngby, Denmark
- 2017 Member of the Evaluation Board of the Leiden Institute of Chemistry, Netherlands
- 2017 - Vice-Chair, Physics Panel, Marie Skłodowska-Curie Individual Fellowships (MSCA-IF) programme of the EU
- 2014 Member of the Distinguished Advisory Board, Institute for Atom-efficient Chemical Transformations (IACT), Argonne National Laboratory, USA
- 2013 - 2015 Member of the User Steering Committee for High Performance Computing in the Federal State of Baden-Württemberg/Germany
- 2019 -
- 2012 - Member of the scientific advisory board and co-spokesperson of the working group “Catalysis” of the Psi-k-Network
- 2010 - Member of the scientific advisory board of the journal *Surface Science*
- 2008 - Member of the scientific advisory board of the journal *Journal of Computational and Theoretical Nanoscience*
- 1993 - Reviewer for numerous journals including Science, Physical Review Letters, Review of Modern Physics, Angewandte Chemie. Journal of the American Chemical Society
- 1993 - Reviewer for science funding organizations including German Science Foundation (DFG), EU FP7-PEOPLE-IEF-IIF-IOF calls, European Research Council (ERC), Austrian Science Fund (FWF), National Science Foundation (NSF, USA), Department of Energy (DOE, USA), Natural Sciences and Engineering Research Council of Canada (NSERC), Netherlands Organisation for Scientific Research (NWO).

MEMBER OF SCIENTIFIC SOCIETIES

- 2023 - Member of the Electrochemical Society (ECS)
- 2018 - Member of the Gesellschaft Deutscher Chemiker (GDCh)
- 2010 - Member of the International Society of Electrochemistry (ISE)
- 2005 - Member of the German Bunsen Society for Physical Chemistry (DBG)
- 2005 - Member of the American Chemical Society (ACS)
- 1991 - Member of the German Physical Society (DPG)

Major COLLABORATIONS

- 2017 - Prof. Dr. Maximilian Fichtner, Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage/Germany, battery modelling
- 2013 - Prof. Dr. R.G. Hennig, University of Florida/USA, implicit solvent models
- 2011 - Prof. Dr. Christof Wöll, Karlsruhe Institute of Technology/Germany, self-assembled monolayers
- 2008 - Prof. Dr. Karsten Reuter, Technical University of Munich/Germany, molecule-surface dynamics
- 2007 - Dr. H.F. Busnengo, CONICET, Rosario/Argentina, molecule-surface dynamics
- 2004 - Prof. Dr. R.J. Behm, Ulm University/Germany, experimental-theoretical collaboration concerning surface science and electrochemistry projects

TRACK RECORD

Publications:

Total number of publications in peer-reviewed journal in the last ten years: 150 articles (out of a total of 315 articles that have been cited more than 13,000 times according to the Web of Science, h-Index: 66, Research-ID: B-4023-2014; Google Scholar: more than 17,700 citations, h-Index: 73)

Invited presentations to peer-reviewed, internationally established conferences

In the last ten years I have been invited to 60 internationally established conferences (out of in total 250 invitations to conferences and seminars in my career).

Major contributions to early careers of excellent researchers

I have been supervising 21 Master students, 24 PhD students and 16 PostDocs. One of them became Associated Professor (Prof. Y. Gohda, University of Tokyo), one of them Assistant Professor (Prof. Xiaohang Lin, Shandong University), seven of them are currently pursuing a scientific career at other scientific institutions (Dr. C. Carbogno, Dr. A. Dianat, Dr. S. Sakong, Dr. A. Roudgar, Dr. Katrin Forster-Tonigold, Dr. Daniela Künzel, Dr. N. Hörmann). Two of the PhD students (Dr. C. Carbogno, Dr. Katrin Forster-Tonigold) were awarded with PhD prizes, one (Dr. Daniela Künzel) was awarded with an Early Career scholarship of the Nüsslein-Vollhard-Foundation.