

## Curriculum Vitae Prof. Dr. Axel Groß, October 2020

### PERSONAL INFORMATION

Groß, Axel

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Nationality: German

Date of birth: 30.12.1961

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### 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

- 1996-2019        Supervision of 21 Master students, 24 PhD students and 16 PostDocs at the Fritz-Haber-Institute, Berlin, the Technical University of Munich, and Ulm University

### TEACHING ACTIVITIES

- 1998-2019        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

- 1999-2020 (Co-)Organization of 18 international workshops, conferences and symposia, four recent ones are given below
- 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
- May 1-4, 2016 Workshop “Elementary Reaction Steps in Electrocatalysis: Theory meets Experiment”, Castle Reisenburg near Ulm
- Mar 30-Apr 4, 2014 Surface Science Section of the Spring Meeting of the German Physical Society in Dresden (832 contributions)

## INSTITUTIONAL RESPONSIBILITIES

- 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 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

- 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: 110 articles (out of a total of 210 articles that have been cited more than 7,800 times according to the Web of Science, h-Index: 52, Research-ID: B-4023-2014; Google Scholar: more than 10,400 citations, h-Index: 60)

### 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 202 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.

### Selected publications

1. "Introducing highly redox-active atomic centers into insertion-type electrodes for Lithium-ion batteries", Y. Ma, Y. Ma, G. Giuli, H. Euchner, A. Groß, G.O. Lepore, F. d'Acapito, D. Geiger, J. Biskupek, U. Kaiser, H.M. Schütz, A. Carlsson, T. Diemant, R.J. Behm, M. Kuenzel, S. Passerini, and D. Bresser, *Adv. Energy Mater.* **10**, 2000783 (2020).
2. "The dynamic nature of CO adlayers on Pt(111) electrodes", Jie Wei, Reihaneh Amirbeigi-arab, Yan-Xia Chen, Sung Sakong, Axel Groß, and Olaf Magnussen, *Angew. Chem. Int. Ed.* **2020**, *59*, 6182-6186.
3. "Towards an atomic-scale understanding of electrochemical interface structure and dynamics, perspective", Olaf Magnussen and Axel Groß, *J. Am. Chem. Soc.* **2019**, *141*, 4777-4790.
4. "Density fluctuations as door-opener for diffusion on crowded surfaces", Ann-Kathrin Henß, Sung Sakong, Philipp K. Messer, Joachim Wiechers, Rolf Schuster, Don C. Lamb, Axel Groß, and Joost Winterlin, *Science* **2019**, *363*, 715-718.

5. "Self-diffusion barriers: possible descriptors for dendrite growth in batteries?", M. Jäckle, K. Helmbrecht, M. Smits, D. Stottmeister, and A. Groß, *Energy Environ. Sci.* **2018**, 11, 3400-3407.
6. "Insight into Sodium Insertion and Storage Mechanism in Hard Carbon", M. Anji Reddy, M. Helen, A. Groß, M. Fichtner, H. Euchner, *ACS Energy Lett.* **2018**, 3, 2851-2857.
7. "The electric double layer at metal-water interfaces revisited", Sung Sakong and Axel Groß, *J. Chem. Phys.* **2018**, 149, 084705.
8. "The importance of the electrochemical environment in the electro-oxidation of methanol on Pt(111)", S. Sakong and A. Groß, *ACS Catalysis* **2016**, 6, 5575 (2016).
9. "Some challenges in the first-principles modeling of structures and processes in electrochemical energy storage and transfer", N. Hörmann, M Jäckle, F. Gossenberger, T. Roman, K. Forster-Tonigold, M. Naderian, S. Sakong, and A. Groß, *J. Power Sources* **2015**, 275, 531-538 (2015).
10. "Microscopic properties of lithium, sodium and magnesium battery anode materials related to possible dendrite growth", M. Jäckle and A. Groß, *J. Chem. Phys.* **2014**, 141, 174710.
11. "Periodic density-functional theory calculations on work-function changes induced by adsorption of halogens on Cu(111)", Tanglaw Roman and Axel Groß, *Phys. Rev. Lett.* **2013**, 110, 156804.
12. "Towards the Microscopic Identification of Anions and Cations at the Ionic Liquid | Ag(111) Interface: A Combined Experimental and Theoretical Investigation", F. Buchner, K. Forster-Tonigold, B. Uhl, D. Alwast, N. Wagner, A. Groß, and R.J. Behm, *ACS Nano* **2013**, 7, 7773-7784.
13. "Hierarchical Interactions and their Influence upon the Adsorption of Organic Molecules on a Graphene Film", M. Roos, D. Künzel, B. Uhl, H. Huang, O.B. Alves, H.E. Hoster, Axel Groß, R.J. Behm, *J. Am. Chem. Soc.* **2011**, 133, 9208-9211.
14. "Challenges in the first-principles description of reactions in electrocatalysis", S. Schnur and A. Groß, *Catal. Today* **2011**, 165, 129-137.
15. "Adsorption of small aromatic molecules on the (111) surfaces of noble metals: a DFT study with semi-empirical corrections for dispersion effects", K. Tonigold and A. Groß, *J. Chem. Phys.* **2010**, 132, 224701.
16. "Properties of metal-water interfaces studied from first principles", S. Schnur and A. Groß, *New J. Phys.* **2009**, 11, 125003.
17. "Six-dimensional quantum dynamics of adsorption and desorption of H<sub>2</sub> at Pd(100): Steering and steric effects", A. Gross, S. Wilke, and M. Scheffler, *Phys. Rev. Lett.* **1995**, 75, 2718-2721.