# Gareth S. Parkinson

Date of Birth: 02 / 06 / 1981 Place of Birth: Darlington, UK <u>Web Site</u> / <u>Google Scholar Profile</u> / <u>ORCID</u>

#### • EDUCATION

2016	Habilitation in Experimental Physics
	Department of Physics, TU Wien, Vienna, Austria
2007	PhD – Surface Studies Using Medium Energy Ion Scattering
	(Advisor D. P. Woodruff)
	Department of Physics, University of Warwick, UK
2004	Masters Degree in Physics (MPhys)
	Department of Physics, University of Warwick, UK

#### • POSITIONS HELD

2021 -	Full Professor of Surface Reactivity
	Institut für Angewandte Physik/ TU Wien
2017 - 2020	Associate Professor
	Institut für Angewandte Physik, TU Wien
2015 - 2017	Assistant Professor (Laufbahnstelle)
	Institut für Angewandte Physik, TU Wien
2010 - 2015	University Assistant
	Institut für Angewandte Physik, TU Wien
2009 - 2010	Postdoctoral Researcher (supervisor U. Diebold)
	Department of Physics, Tulane University, New Orleans LA, USA
2007 - 2009	Postdoctoral Researcher (supervisor B.D. Kay)
	Pacific Northwest National Laboratory (PNNL), Richland WA, USA

## **RESEARCH INTERESTS**

Since my appointment at the TU Wien in 2010, my research group has studied the atomic-scale processes underlying reactivity on metal-oxide surfaces. Iron oxides have been a major focus of my work because they are omnipresent in the natural environment and find widespread applications in technology. The work has been highly successful including papers in *Science, Nature Materials, PNAS; Physical Review Letters, Angewandte Chemie, ACS Nano, JACS*, and the *Journal of Physical Chemistry*. The highlight was our discovery that the Fe<sub>3</sub>O<sub>4</sub>(001) surface stabilizes arrays of single metal adatoms (Au, Ag, Pd, Ni...) to high temperatures, which makes an ideal model system to study fundamental aspects of "single-atom" catalysis (SAC). In 2015 I was awarded the FWF START prize (€ 1.2M over 6 years) to study the mechanisms of SAC. This work has generated much interest, illustrated by the invitations I have received to international conferences and seminars. In 2016, I published a single author review of Iron Oxide Surfaces in surface science reports. In 2020 I was awarded an ERC consolidator grant to expand my work on SAC to more realistic supports and atmospheres.

#### • PUBLICATION SUMMARY

81 articles in peer reviewed journals: 13 first author, 21 senior author. 3 single author Articles include: 2 Science, 2 PNAS, 3 Nature Materials, 4 Angewandte Chemie, 4 Physical Review Letters, 1 JACS, 2 ACS Nano, 2 ACS Catalysis Google scholar h-index – 32, ≈3600 total citations

## • AWARDS

- 2022 Elected as AVS fellow
  2022 Young Innovator Award in Nano Research (Nanocatalysis)
  2020 ERC Consolidator grant (€2m over 5 years)
  2018 Gaede-Prize of the German Physical Society (DPG) "...For his excellent experimental work on iron oxide surfaces as model systems for single atom catalysis." One prize annually for outstanding work in vacuum-related research.
  2017 Kardinal Innitzer Förderungspreis (Awarded annually for best habilitation thesis in Austria)
- 2015 FWF START Prize (similar to ERC starting grant, ca. 8 per year in all of research, comes with €1.2 million in unrestricted research funds)
- 2013 Department of Energy Office of Science Postdoctoral Researcher Competition

# • **PROFESSIONAL SERVICE**

- 2019 Elected to IUVSTA Surface Science Division committee
- 2019 Elected IUVSTA representative for Austria by the Austrian Vacuum Society (BWG)
- 2019 Joined committee for "Fundamental Discoveries in Heterogeneous Catalysis Focus Session" at AVS
- 2018 Appointed representative for the surface science division of the Austrian Physics Society (ÖPG)
- 2017 2019 Elected to the board of the Austrian Chemical-Physics Society (CPG)
- 2017 2019 Elected to AVS surface science division executive board
- 2011 2012 Member of Editorial Board, Energy Frontier Research Centre Newsletter

## • INVITED TALKS

**46 invited talks** at international conferences, workshops and summer schools, including 2 keynote lectures, 3 pleanary lectures and the **"Future Stars of the AVS" Symposium"** (see full list for details).

24 invited seminars and colloquia at universities and research institutions (see full list for details).

## • CONFERENCE ORGANIZATION

2022	Organizing symposium on Single Atom Catalysis at DPG 2022 Sprig Meeting
2020-2022	Co-organizing "Fundamentals of heterogeneous catalysis" focus session at AVS 67 (cancelled due to Covid-19)
2019-2022	Organized surface science division sessions for joint ÖPG/SPG national meeting
2019	Co-organized "Fundamental Aspects of Materials Degradation" symposium at AVS 66 with Marcus Valtiner (TU Wien)
2017	Co-organized fundamentals of metal-oxide surface chemistry at DPG spring meeting with Joachim Paier (Helmholtz Univ, Berlin)

## • INSTITUTIONAL RESPONSIBILITIES

- 2019 Ersatzmitglied for Appointment Committee Professorship "Experimentelle Quantentechnologie"
- Hauptmitglied for IAP in the TU Wien Physics Faculty Council (Fakultätsrat)
  Chair of "Vienna young scientists symposium" Catalysis section
- 2016 2019 IAP "Mittelbau" representative on the TU Wien Physics Faculty Council
- 2016 2018 Member in 3 Habilitation committees (Jan Tomczak, Stijn Mertens, Martin Setvin)

# • **RESEARCH FUNDING**

Title	Funding Agency	Amount	Duration	Role
SFB: Taming complexity in Materials Modelling	Austrian Science Foundation	€4.8M (€430k to GSP)	2021-2026	PI
ERC Consolidator Grant	ERC	€2.0M	2020-2025	PI
FWF "START" Prize	Austrian Science Foundation	€1.2M	2015-2021	PI
Surface Science of Magnetite	Austrian Science Foundation – single investigator project	€152k	2013-2016	PI
TU-d Doctoral College	TU Wien	€76,5k (one PhD student)	2016-2019	PI
SFB 'Functional Oxide Surfaces and Interfaces, <u>FOXSI</u> '	Austrian Science Foundation	€2M	2015-2019	Co-Applicant
An Artificial Leaf: a photo- electro-catalytic cell from earth-abundant materials for sustainable solar production of CO <sub>2</sub> -based chemicals and fuels (participant)	H2020 (EU)	€7.98M; (€547,612€ to TU Wien)	2016-2019	Participant
An Apparatus for Investigating Organic Molecules on Oxide Surfaces	TU Wien	€141k	2012-2014	Co-Applicant

# • PENDING FUNDING

Title	Funding Agency	Amount	Duration	Role
TU-dx – Towards applications of 2D materials and their heterostructures	Austrian Science Foundation – Docfunds Program	150k to GSP	2023-2027	PI
Advanced Single Atom Electrochemistry	EU - Marie Curie Fellowship for Hao Yin (EPFL)	300k	2023-2025	Supervisor
Cluster of Excellence	Austrian Science Foundation	€34.4M (circa. €700k to GSP)	2023-2028	PI

# • INVITED TALKS AT INTERNATIONAL MEETINGS

- 1. ACS Spring 2012 National Meeting and Exposition San Diego, March 25-29, 2012
- 2. Nature Conference "Frontiers in Electronic Materials", June 17-20, 2012, Aachen, Germany
- 3. SPIE Optics & Photonics San Diego, USA, August 12-16, 2012
- 4. IUPAC 8th International Conference on Novel Materials and their Synthesis (NMS-VIII), Xi'An, China, 14 to 19 October, 2012
- 5. 28<sup>th</sup> International Workshop on Novel Materials and superconductors, Planneralm, Austria, February 9 - 16, 2013
- 6. ACS Spring 2013 National Meeting and Exposition New Orleans, April 7-11, 2013
- 7. Austrian Physical Society (ÖPG) Meeting, Linz Austria, 3-6 September 2013
- 8. 3<sup>rd</sup> International Conference on Physics at Surfaces and Interfaces (PSI2014), Puri, India, Feb 24-28 2014
- 9. 79<sup>th</sup> DPG Annual Meeting and DPG Spring Meeting (DPG-Frühjahrstagung), Berlin (TU), 15-20 March 2015
- 10. Nanoforum 2015, June 8–9, 2015, University Linz
- 11. ACS Fall 2015 National Meeting and Exposition Boston, August 16-20, 2015
- 12. CRC 1109 Summer School, Berlin, Germany, 03.09.2015
- 13. International SFB FOXSI Symposium, TU Wien, 12.5.2015
- 14. AMISPEC Workshop, Central European Institute of Technology, March 8 2016
- 15. ACS Spring 2016 National Meeting and Exposition San Diego, March 13-17, 2016
- 16. IUVSTA 76 Workshop, Avilla, Spain, July 2016
- 17. (**Keynote Lecture**) International Symposium on Single-Atom Catalysis, Dalian, China, June 30-July 2, 2016
- 18. (Keynote Lecture) 20th International Vacuum Congress (IVC-20), Busan, Korea August 21 to 26, 2016.
- 19. ECOSS 32. Grenoble France, 28th August -2nd September 2016
- 20. Summer School of the Oldenburger LandesgraduiertenKolleg in Elstal, Germany. September 12-14, 2016.
- 21. Austrian Physical Society (ÖPG) Meeting, Vienna Austria, 3-6 September 2016
- 22. AVS 63rd International Symposium and Exhibition, Nashville November 6-11, 2016
- 23. 2016 Fall MRS Meeting, Boston, November 27- December 2, 2016
- 24. IUVSTA International Summer School on Physics at Nanoscale, June 10th-June 17th 2017, Devět Skal, Czech Republic
- 25. 5th International Conference on Chemical Bonding, ICCB, Kauai, Hawaii, June 22-26, 2017
- 26. E-MRS 2017 Fall Meeting, Warsaw Poland, September 18-21, 2017.
- 27. (**Plenary Lecture**) 82<sup>nd</sup> Annual Meeting of the German Physical Society (DPG-Frühjahrstagung), Berlin (TU), 11-16 March 2018
- 28. STINT workshop, Fort Myers, Florida, USA. 3-6 April 2018
- 29. (**Plenary Lecture**) 2nd International Symposium on Single Atom Catalysis, Beijing, China 15-18 July, 2018
- 30. SFB 986 Summer School, Hamburg, Germany, 9-13 July 2018
- 31. Telluride Workshop on Semiconductor Surface Chemistry, Telluride, Colorado July 2018
- 32. Deutsch-Brasilianischer Workshop, Bad Dürkheim Germany, 23.9 28.9 2018
- 33. AVS 65th International Symposium and Exhibition Long Beach California "Future Stars of the AVS" Symposium
- 34. Gordon Research Conference on "Chemical Reactions at Surfaces" Ventura CA, Feb 2019
- 35. IWSP Workshop, Wrocklaw Poland, 24-28 June 2019
- 36. Festkorper Analytic Symposium (FKA-20), Wien, Austria 3rd July 2019
- 37. AVS 66th International Symposium and Exhibition Columbus Ohio October 2019
- 38. Materials Research Meeting (MRM) 2019 December 10-14, 2019, Yokohama, Japan
- 39. (Plenary Lecture) International workshop on oxide surfaces (IWOX) Lake Placid NY, USA, Jan 2020
- 40. DPG Spring Meeting (DPG-Frühjahrstagung), Dresden, 15-20 March 2020 conference cancelled due to Covid-19
- 41. ACS Spring Meeting, Philadeplhia, USA conference cancelled due to Covid-19

- 42. ACS Fall Meeting, San Francisco, USA conference cancelled due to Covid-19
- 43. Summer school in Photo- and electro-catalysis at the atomic scale (PECAS), San Sebastian, Spain, June 22-25 2021 postponed to 2022.
- 44. Multiscale approaches for modeling water splitting with nanocrystals, COST action online Workshop. 16.02.2021
- 45. Surface Science Discussions 2022, Online workshop (January 2022)
- 46. LINXS Catalysis Workshop, June 30, 2022, Lund, Sweden

#### • INVITED TALKS AT UNIVERSITIES AND RESEARCH INSTITUTIONS

- 1. University of Cambridge, UK (2007)
- 2. Pacific Northwest National Laboratory (2009)
- 3. Ludwig-Maximilians University, Munich (2010)
- 4. Louisiana State University (2012)
- 5. Georgia Institute of Technology (2012)
- 6. Max Plank Institute for Solid State Research Stuttgart (2013)
- 7. TU Wien, IAP Seminar (2013)
- 8. Max Plank Institute for Microstructure Physics, Halle Saale (2014)
- 9. Chemisch Phisikalishe Gesellschaft (July 2015)
- 10. TU Munich (November 2015)
- 11. TU Graz (May 2016)
- 12. York University (June 2016)
- 13. Tufts University (December 2016)
- 14. Harvard University (December 2016)
- 15. PNNL (June 2017)
- 14. TU Hamburg (April 2018)
- 15. Aarhus iNano centre (June 2018)
- 16. TU Wien Institute of Theoretical Physics (July 2018)
- 17. University of Marburg (May 2019)
- 18. University of Warwick (June 2019)
- 19. University of Duisburg-Essen (November 2019)
- 20. Tufts University (October 2020)
- 21. Michigan Technological University (October 2020)
- 22. Chalmers University (November 2021)
- 23. University of Zurich (May 2022)
- 24. Peking University (June 2022)

#### • PhD STUDENT SUPERVISION

Ongoing: David Rath (2022), Lena Haager (2023), Ali Rafsanjani (2023), Panukorn Sombut (2023).

September 202	21 Florian Kraushofer, Institute of Applied Physics, TU Wien
-	"Iron Oxide Surfaces as Support Materials for Single Atom Catalysis" Currently postdoc at TU Munich with Barbara Lechner
June 2020	Zdenek Jakub, Institute of Applied Physics, TU Wien

- "Surface Science Studies of Iron Oxides as Model Catalyst Supports" Obtained a Marie Curie Grant to work as postdoc at CEITEC, Brno
- May 2019Jan Hulva, Institute of Applied Physics, TU Wien"Studies of adsorption on Fe<sub>3</sub>O<sub>4</sub>(001) using molecular beams
- April 2019Jiri Pavelec, Institute of Applied Physics, TU Wien<br/>"Surface Chemistry Setup and Adsorption of CO2 on Fe<sub>3</sub>O<sub>4</sub>(001)"

Currently Assistant Professor at TU Vienna.

- October 2016 Oscar Gamba, Institute of Applied Physics, TU Wien "Surface Chemistry of  $Fe_3O_4(001)$ " Assistant professor in Colombia
- August 2016Roland Bliem, Institute of Applied Physics, TU Wien<br/>Awarded the Christian Doppler Prize for his PhD thesis<br/>"Single Metal Adatoms at the Reconstructed Fe<sub>3</sub>O<sub>4</sub>(001) Surface"<br/>Currently Assistant professor at the University of Amsterdam
- 2013 Zdenek Novotny, Institute of Applied Physics, TU Wien. Awarded Loschmidt Prize of the CPG for his thesis *"The Reconstructed Fe<sub>3</sub>O<sub>4</sub>(001) Surface as an Adsorption Template"* Currently a staff scientist at PSI, Zurich, Switzerland.

#### • PhD OPPONENT FOR:

2022	Moritz Eder (supervisor Ueli Heiz) – TU Munich Germany
2018	Bjorn Arndt (supervisor Andreas Stierle) – DESY, Germany
2018	Jakob Fester (supervisor Jeppe Lauritsen) – Aarhus University, Denmark
2017	Brian Walls (supervisor Igor Shvets) – Trinity College, Dublin, Ireland
2014	Matteo Monti (supervisor Juan de la Figuera) – CISC Madrid, Spain

#### • MAJOR COLLABORATIONS

Prof. Cesare Franchini (University of Vienna, Austria) – Theoretical modelling (DFT)
Prof. Peter Blaha (TU Wien, Austria) - Theoretical modelling (DFT)
Prof. Florian Libisch (TU Wien, Austria) – DFT with the "embedding" approach
Prof. Edvin Lundgren (Lund, Sweden) – Surface x-ray diffraction
Prof. Andreas Stierle (DESY, Germany) – Surface x-ray diffraction
Prof. Lutz Hammer – (Erlangen, Germany) – Low energy electron diffraction
Dr. Zdenek Dohnalek (PNNL, USA) - SAC studies on Fe3O4(001)
Dr. David Duncan (Diamond, UK) – Synchrotron studies (quantitative structural determination)
Prof. Juan de la Figuera (CISC Madrid) – Low energy electron microscopy and magnetite in general.
Prof. Prof. Barbara Lechner (TU Munich) – High temperature and ambient pressure STM

Ten Most Important Research Papers:

- Matthias Meier, Jan Hulva, Zdenek Jakub, Florian Kraushofer, Mislav Bobić, Roland Bliem, Martin Setvin, Michael Schmid, Ulrike Diebold, Cesare Franchini and Gareth S. Parkinson "CO oxidation by Pt<sub>2</sub>/Fe<sub>3</sub>O<sub>4</sub>: metastable dimer and support configurations facilitate lattice oxygen extraction"
   Science Advances – In press (2022)
- Jan Hulva, Matthias Meier, Roland Bliem, Zdenek Jakub, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson "Unravelling CO Adsorption on Model Single-Atom Catalysts" Science 371 (2021) 375-379 – <u>https://doi.org/10.1126/science.abe5757</u>
- Zdenek Jakub, Jan Hulva, Matthias Meier, Roland Bliem, Florian Kraushofer, Martin Setvin, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson *"Local Structure and Coordination Effects Define Adsorption in a Model Ir<sub>1</sub>/Fe<sub>3</sub>O<sub>4</sub> Single-Atom Catalyst"
   Angewandte Chemie International Edition 58, 13961-13968 (2019) https://doi.org/10.1002/anie.201907536*

- Matthias Meier, Jan Hulva, Zdeněk Jakub, Jiří Pavelec, Martin Setvin, Roland Bliem, Michael Schmid, Ulrike Diebold, Cesare Franchini, and Gareth S. Parkinson
   *"Water Agglomerates on Fe<sub>3</sub>O<sub>4</sub>(001)"* PNAS 115, E5642-E5650 (2018) <u>https://doi.org/10.1073/pnas.1801661115</u>
- 5. Roland Bliem, Jessi van der Hoeven, Adam Zavodny, Oscar Gamba, Jiri Pavelec, Petra E de Jongh, Michael Schmid, Ulrike Diebold, Gareth S Parkinson
  "Dual role of CO in the stability of sub-nano Pt clusters at the Fe<sub>3</sub>O<sub>4</sub>(001) surface"
  PNAS 113, 8921 (2016) <u>http://dx.doi.org/10.1073/pnas.1605649113</u>
- 6. Gareth S. Parkinson
   *"Iron Oxide Surfaces"* Surface Science Reports 71 (2016) 272 <u>10.1016/j.surfrep.2016.02.001</u>
- Roland Bliem, Jessi van der Hoeven, Adam Zavodny, Oscar Gamba, Jiri Pavelec, Petra E de Jongh, Michael Schmid, Ulrike Diebold, Gareth S Parkinson
  "An Atomic-Scale View of CO and H<sub>2</sub> Oxidation on a Pt/Fe<sub>3</sub>O<sub>4</sub> Model Catalyst"
  Angewandte Chemie International Edition 54 (47), 13999-14002 (2016)
  http://dx.doi.org/10.1002/anie.201507368
- Roland Bliem, Eamon McDermott, Pascal Ferstl, Martin Setvin, Oscar Gamba, M. Alexander Schneider, Michael Schmid, Ulrike Diebold, Peter Blaha, Lutz Hammer, Gareth S. Parkinson "Subsurface Cation Vacancy Stabilization of the Magnetite (001) Surface" Science 346 (2014) 1215-1218. - <u>http://dx.doi.org/10.1126/science.1260556</u>
- 9. G. S. Parkinson, Z. Novotny, G. Argentero, M. Schmid, J. Pavelec, R. Kosak, P. Blaha, U. Diebold.
  "CO Induced Adatom Sintering in a Pd/Fe<sub>3</sub>O<sub>4</sub> Model Catalyst" Nature Materials, 12, 724 (2013) - <u>http://dx.doi.org/10.1038/nmat3667</u>
- Z. Novotny, G. Argentero, Z. Wang, M. Schmid, U. Diebold, G.S. Parkinson.
   *"Ordered Array of Single Adatoms with Remarkable Thermal Stability: Au/Fe<sub>3</sub>O<sub>4</sub>(001)"* Phys. Rev. Lett., 108, 216103 (2012) <u>http://dx.doi.org/10.1103/PhysRevLett.108.216103</u>