

## Gareth S. Parkinson – Full Publication List

### Book Chapters

1. G. S. Parkinson, U. Diebold, J. K. Tang, and L. Malkinski, in *Magnetic Materials*, edited by L. Malkinski (InTech, 2012)
2. G.S. Parkinson, U. Diebold, “*Adsorption at metal oxide surfaces*”, published in “*Surface and Interface Science*” edited by Klaus Wandelt (Wiley, 2016)

### Papers in Peer Reviewed Journals

88. Lena Puntischer, Panukorn Sombut, Chunlei Wang, Manuel Ulreich, Jiri Pavelec, Ali Rafsanjani-Abbasi, Matthias Meier, Adam Lagin, Martin Setvin, Ulrike Diebold, Cesare Franchini, Michael Schmid and Gareth S. Parkinson  
“*A Multi-Technique Study of C<sub>2</sub>H<sub>4</sub> Adsorption on Fe<sub>3</sub>O<sub>4</sub>(001)*”  
The Journal of Physical Chemistry C 127, 18378–18388 (2023)  
<https://doi.org/10.1021/acs.jpcc.3c03684>
87. Nicolo Comini, John Diulus, Gareth Parkinson, Jürg Osterwalder, Zbynek Novotny  
“*Stability of Iridium Single Atoms on Fe<sub>3</sub>O<sub>4</sub>(001) in the mbar Pressure Range*”  
The Journal of Physical Chemistry C 127 19097–19106 (2023)  
<https://doi.org/10.1021/acs.jpcc.3c03097>
86. Jesús Redondo, Jan Michalička, Florian Kraushofer, Giada Franceschi, Břetislav Šmid, Nishant Kumar, Ondřej Man, Matthias Blatnik, Dominik Wrana, Benjamin Mallada, Martin Švec, Gareth S. Parkinson, Martin Setvin, Michele Riva, Ulrike Diebold, Jan Čechal  
“*Hematite  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) in Top and Side View: Resolving Long-Standing Controversies about Its Surface Structure*”  
Advanced Materials Interfaces. In Press 2023  
<https://doi.org/10.1002/admi.202300602>
85. Florian Kraushofer, Matthias Meier, Zdeněk Jakub, Johanna Hütner, Jan Balajka, Jan Hulva, Michael Schmid, Cesare Franchini, Ulrike Diebold, Gareth S Parkinson  
“*Oxygen-Terminated (1 × 1) Reconstruction of Reduced Magnetite Fe<sub>3</sub>O<sub>4</sub>(111)*”  
The Journal of Physical Chemistry Letters 14, 3258-3265 (2023)  
<https://doi.org/10.1021/acs.jpcclett.3c00281>
84. L Puntischer, K Daninger, M Schmid, U Diebold, GS Parkinson  
“*A study of Pt, Rh, Ni and Ir dispersion on anatase TiO<sub>2</sub> (101) and the role of water*”  
Electrochimica Acta 449, 142190 (2023)  
<https://doi.org/10.1016/j.electacta.2023.142190>
83. Michael Schmid, Gareth S. Parkinson, Ulrike Diebold  
“*Analysis of Temperature-Programmed Desorption via Equilibrium Thermodynamics*”  
ACS Physical Chemistry Au (2022)  
<https://doi.org/10.1021/acsphyschemau.2c00031>
82. Gareth S. Parkinson, P. Christopher  
“*Preface to the Special Issue on Single Atom Catalysis*”  
Topics in Catalysis, 1-2 (2022)  
<https://doi.org/10.1007/s11244-022-01740-0>
81. P Sombut, L Puntischer, M Atzmueller, Z Jakub, M Reticioli, M Meier, Gareth S Parkinson, Cesare Franchini

- “Role of Polarons in Single-Atom Catalysts: Case Study of  $Me_1$  [ $Au_1$ ,  $Pt_1$ , and  $Rh_1$ ] on  $TiO_2$  (110)”  
 Special issue of Topics in Catalysis (2022)  
<https://doi.org/10.1007/s11244-022-01651-0>
80. Florian Kraushofer and Gareth S. Parkinson  
 “Single Atom Catalysis: Lessons from Model Systems”  
 Invited Review - Chem. Rev. 122, 18, 14911–14939 (2022)  
<https://doi.org/10.1021/acs.chemrev.2c00259>
79. 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  $Pt_2/Fe_3O_4$ : metastable dimer and support configurations facilitate lattice oxygen extraction”  
 Science Advances 8 (13), eabn4580 (2022)  
<https://doi.org/10.1038/s41467-021-26601>
78. Florian Kraushofer, Lena Haager, Moritz Eder, Ali Rafsanjani-Abbasi, Zdeněk Jakub, Giada Franceschi, Michele Riva, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S Parkinson  
 “Single Rh Adatoms Stabilized on  $\alpha\text{-}Fe_2O_3(1\bar{1}02)$  by Coadsorbed Water”  
 ACS energy letters 7, 375-380 (2021)  
<https://doi.org/10.1021/acseenergylett.1c02405>
77. Gareth S. Parkinson  
 “Adding Oxides to the 2D Toolkit”  
 Nature Materials - News and Views  
<https://doi.org/10.1038/s41563-021-01048-6>
76. Zdenek Jakub, Matthias Meier, Florian Kraushofer, Jan Balajka, Jiri Pavelec, Michael Schmid, Cesare Franchini, Ulrike Diebold, Gareth S. Parkinson  
*Rapid oxygen exchange between hematite and water vapor*  
 Nature Communications 12, 6488 (2021)  
<https://doi.org/10.1038/s41467-021-26601>
75. Francesca Mirabella, Matthias Müllner, Thomas Touzalin, Michele Riva, Zdenek Jakub, Florian Kraushofer, Michael Schmid, Marc T.M. Koper, Gareth S. Parkinson, Ulrike Diebold  
 “Ni-modified  $Fe_3O_4(001)$  surface as a simple model system for understanding the oxygen evolution reaction”  
 Electrochimica Acta Volume 389, 138638 (2021)  
<https://doi.org/10.1016/j.electacta.2021.138638>
74. Florian Kraushofer, Nikolaus Resch, Moritz Eder, Ali Rafsanjani-Abbasi, Sarah Tobisch, Zdenek Jakub, Giada Franceschi, Michele Riva, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
 “Surface Reduction State Determines Stabilization and Incorporation of Rh on  $\alpha\text{-}Fe_2O_3(1\bar{1}\bar{0}2)$ ”  
 Advanced Materials Interfaces special issue on Single-Atom Catalysis, in press  
 Article selected for cover of the special issue  
<https://doi.org/10.1002/admi.202001908>
73. 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  
<https://doi.org/10.1126/science.abe5757>

72. Jakob Timmermann, Florian Kraushofer, Nikolaus Resch, Peigang Li, Yu Wang, Zhiqiang Mao, Michele Riva, Yonghyuk Lee, Carsten Staacke, Michael Schmid, Christoph Scheurer, Gareth S. Parkinson, Ulrike Diebold, and Karsten Reuter  
*“IrO<sub>2</sub> Surface Complexions Identified Through Machine Learning and Surface Investigations”*  
 Phys. Rev. Lett. 125 (2020) 206101  
<https://doi.org/10.1103/PhysRevLett.125.206101>
71. Doris Grumelli, Tim Wiegmann, Sara Barja, Finn Reikowski, Fouad Maroun, Jan Balajka, Gareth S. Parkinson, Ulrike Diebold, Philippe Allongue, Klaus Kern, Olaf Magnussen  
*“Electrochemical Stability of the Reconstructed Fe<sub>3</sub>O<sub>4</sub>(001) Surface”*  
 Angewandte Chemie, 59, 21904-21908 (2020).  
<https://doi.org/10.1002/anie.202008785>
70. Francesca Mirabella, Jan Balajka, Jiri Pavelec, Markus Göbel, Florian Kraushofer, Michael Schmid, Gareth Parkinson, and Ulrike Diebold  
*“Atomic-Scale Studies of Fe<sub>3</sub>O<sub>4</sub>(001) and TiO<sub>2</sub>(110) Surfaces Following Immersion in CO<sub>2</sub>-Acidified Water”*  
 ChemPhysChem 21 (2020) 1788-1796  
<https://doi.org/10.1002/cphc.202000471>
69. Giada Franceschi, Florian Kraushofer, Matthias Meier, Gareth S. Parkinson, Michael Schmid, Ulrike Diebold, and Michele Riva  
*“A model system for photocatalysis: Ti-doped Fe<sub>2</sub>O<sub>3</sub>(1-102) single-crystalline films”*  
 Chemistry of Materials, 32, 9, 3753–3764 (2020)  
<https://doi.org/10.1021/acs.chemmater.9b04908>
68. Björn Arndt, Barbara A. J. Lechner, Alexander Bourgund, Elin Grånäs, Marcus Creutzburg, Konstantin Krausert, Vedran Vonk, Jan Hulva, Gareth S. Parkinson, Michael Schmid, Friedrich Esch, Andreas Stierle  
*“Order-disorder phase transition of the subsurface cation vacancy reconstruction on Fe<sub>3</sub>O<sub>4</sub>(001)”*  
 Physical Chemistry Chemical Physics, 22, 8336-8343 (2020)  
 Selected for “2020 PCCP Hot Article Collection”  
<https://doi.org/10.1039/D0CP00690D>
67. Zdenek Jakub, Jan Hulva, Paul T. P. Ryan, David A. Duncan, David J. Payne, Roland Bliem, Manuel Ulreich, Patrick Hofegger, Florian Kraushofer, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
*“Adsorbate-induced structural evolution changes the mechanism of CO oxidation on a Rh/Fe<sub>3</sub>O<sub>4</sub>(001) model catalyst”*  
 Nanoscale 12, 5866 – 5875 (2020)  
<https://doi.org/10.1039/C9NR10087C>
66. Matthew D. Marcinkowski, Kræn C. Adamsen, Nassar Doudin, Marcus A. Sharp, R. Scott Smith, Yang Wang, Stefan Wendt, Jeppe V. Lauritsen, Gareth S. Parkinson, Bruce D. Kay Zdenek Dohnálek  
*“Adsorption and reaction of methanol on Fe<sub>3</sub>O<sub>4</sub>(001)”*  
 J. Chem. Phys. 152, 064703 (2020)  
<https://doi.org/10.1063/1.5139418>
65. P. T. P. Ryan, M. Meier, Z. Jakub, J. Balajka, J. Hulva, D. J. Payne, T.-L. Lee, C. Franchini, F. Allegretti, G. S. Parkinson, D. A. Duncan  
*“Probing structural changes upon carbon monoxide coordination to single metal adatoms”*  
 J. Chem. Phys. 152, 051102 (2020);  
<https://doi.org/10.1063/1.5137904>

64. Florian Kraushofer, Francesca Mirabella, Jian Xu, Jiří Pavelec, Jan Balajka, Matthias Müllner, Nikolaus Resch, Zdeňek Jakub, Jan Hulva, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
 “Self-limited Growth of an Oxyhydroxide Phase at the  $Fe_3O_4(001)$  Surface in Liquid and Ambient Pressure Water”  
 The Journal of Chemical Physics, 151 (15), 154702 (2019)  
<https://doi.org/10.1063/1.5116652>
63. Nassar Doudin, Simuck F. Yuk, Matthew D. Marcinkowski, Manh-Thuong Nguyen, Jin-Cheng Liu, Yang Wang, Bruce D. Kay, Jun Li, Vassiliki-Alexandra Glezakou, Gareth S. Parkinson, Roger Rousseau, Zdenek Dohnálek  
 “Hydrogen Activation and Spillover on Single Palladium Atoms Supported on the  $Fe_3O_4(001)$  Surface”  
 ACS Catalysis 9, 7876-7887 (2019)  
<https://doi.org/10.1021/acscatal.9b01425>
62. Alexander Bourgund, Barbara A. J. Lechner, Matthias Meier, Cesare Franchini, Gareth S. Parkinson, Ueli Heiz and Friedrich Esch  
 “Influence of Local Defects on the Dynamics of O-H Bond Breaking and Formation on a Magnetite Surface”  
 The Journal of Physical Chemistry C, 123, 19742-19747 (2019)  
<https://doi.org/10.1021/acs.jpcc.9b05547>
61. 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  $Ir_1/Fe_3O_4$  Single-Atom Catalyst”  
 Angewandte Chemie International Edition 58, 13961-13968 (2019)  
<https://doi.org/10.1002/anie.201907536>
60. Zdenek Jakub, Jan Hulva, Francesca Mirabella, Florian Kraushofer, Ulrike Diebold, Gareth S. Parkinson  
 “Nickel Doping Enhances the Reactivity of  $Fe_3O_4(001)$  to Water”  
 Journal of Physical Chemistry C 2019,12, 15038-15045  
<https://doi.org/10.1021/acs.jpcc.9b02993>
59. Eman Zaki, Zdenek Jakub, Francesca Mirabella, Gareth S. Parkinson, Shamil Shaikhutdinov, and Hans-Joachim Freund  
 “Water Ordering on the Magnetite  $Fe_3O_4$  Surfaces”  
 J. Phys. Chem. Lett., 2019, 10, pp 2487–2492  
<https://doi.org/10.1021/acs.jpcc.9b00773>
58. G. S. Parkinson.  
 Invited Perspective: “Single-Atom Catalysis: How Structure Influences Catalytic Performance”  
 Catalysis Letters 149, 1137 (2019)  
<https://doi.org/10.1007/s10562-019-02709-7>
57. Z. Jakub, F. Kraushofer, M. Bichler, J. Balajka, Jan, J. Hulva, J. Pavelec, I. Sokolović, M. Müllner, M. Setvin, M. Schmid, U. Diebold, P. Blaha, G. S. Parkinson  
 “Partially Dissociated Water Dimers at the Water–Hematite Interface”  
 ACS Energy Letters 4, 390–396 (2019)  
<https://doi.org/10.1021/acsenerylett.8b02324>
56. Matthias Müllner, Michele Riva, Florian Kraushofer, Michael Schmid, Gareth S. Parkinson\*, Stijn F.L. Mertens and Ulrike Diebold

- “Stability and catalytic performance of reconstructed  $Fe_3O_4(001)$  and  $Fe_3O_4(110)$  surfaces during oxygen evolution reaction” -JPCC Festschrift in honor of H.J. Freund and J. Sauer  
 J. Phys. Chem. C, Article ASAP  
<https://doi.org/10.1021/acs.jpcc.8b08733>
55. Peter Lackner, Jan Hulva, Eva-Maria Köck, Wernfried Mayr-Schmölzer, Joong Il J Choi, Simon Penner, Ulrike Diebold, Florian Mittendorfer, Josef Redinger, Bernhard Klötzer, Gareth S Parkinson, Michael Schmid  
 “Water adsorption at zirconia: from the  $ZrO_2(111)/Pt_3Zr(0001)$  model system to powder samples”  
 J. Mater. Chem. A 6, 17587-17601 (2018)  
<https://doi.org/10.1039/C8TA04137G>
54. 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  $Fe_3O_4(001)$ ”  
 PNAS 115, E5642-E5650 (2018)  
<https://doi.org/10.1073/pnas.1801661115>
53. Matthias Meier, Zdeněk Jakub, Jan Balajka, Jan Hulva, Roland Bliem, Pardeep K. Thakur, Tien-Lin Lee, Cesare Franchini, Michael Schmid, Ulrike Diebold, Francesco Allegretti, David A. Duncan and Gareth S. Parkinson  
 “Benchmarking the Active-Site Geometry in a Model Single-Atom Catalyst: NIXSW Studies of Copper and Silver Adatoms on Magnetite”  
 Nanoscale, 2018, 10, 2226 – 2230  
<https://doi.org/10.1039/C7NR07319D>
52. Florian Kraushofer, Zdenek Jakub, Magdalena Bichler, Jan Hulva, Peter Drmota, Michael Weinold, Michael Schmid, Martin Setvin, Ulrike Diebold, Peter Blaha, Gareth S. Parkinson  
 “Atomic-Scale Structure of the Hematite  $\alpha-Fe_2O_3(11\bar{0}2)$  “R-cut” Surface”  
 J. Phys. Chem. C, 2018, 122 (3), pp 1657–1669  
<http://dx.doi.org/10.1021/acs.jpcc.7b10515>
51. M. Setvin, X. Shi, J. Hulva, T. Simschitz, G.S. Parkinson, M. Schmid, C. Di Valentin, A. Selloni, U. Diebold  
 “Methanol on Anatase  $TiO_2(101)$ : Mechanistic Insights into Photocatalysis”  
 ACS Catalysis 7, 7081 (2017)  
<http://dx.doi.org/10.1021/acscatal.7b02003>
50. J. Hulva, Z. Jakub, Z. Novotny, N. Johansson, J. Knudsen, J. Schnadt, M. Schmid, U. Diebold, G.S. Parkinson  
 “Adsorption of CO on the  $Fe_3O_4(001)$  Surface”  
 Miquel Salmeron Festschrift Issue - Journal of Chemistry B (2017)  
<http://dx.doi.org/10.1021/acs.jpcc.7b06349>
49. G.S. Parkinson  
 Invited Perspective Article: “Single Atom Catalysis: The Surface Science Approach”  
 Chinese Journal of Catalysis 38 (2017)  
<http://www.cjcatal.org/CN/article/downloadArticleFile.do?attachType=PDF&id=22213>
48. M. Setvin, J. Hulva, H. Wang, T. Simschitz, M. Schmid, G.S. Parkinson, C. Di Valentin, A. Selloni, U. Diebold  
 “Formaldehyde Adsorption on the Anatase  $TiO_2(101)$  Surface: Experimental and Theoretical Investigation”  
 The Journal of Physical Chemistry C 121 (16), 8914-8922 (2017)

<http://dx.doi.org/10.1021/acs.jpcc.7b01434>

47. M. Setvin, M. Wagner, M. Schmid, G.S. Parkinson, U. Diebold,  
“*Surface point defects on bulk oxides: atomically-resolved scanning probe microscopy*”  
Chemical Society Reviews 46 1772-1784 (2017)  
DOI: <http://dx.doi.org/10.1039/C7CS00076F>
46. M. Setvin, J. Hulva, G.S. Parkinson, M. Schmid, U. Diebold  
“*Electron transfer between anatase TiO<sub>2</sub> and an O<sub>2</sub> molecule directly observed by atomic force microscopy*”  
Proceedings of the National Academy of Sciences 114 E2556-E2562 (2017)  
DOI: <http://dx.doi.org/10.1073/pnas.1618723114>
45. Jiri Pavelec, Jan Hulva, Daniel Halwidl, Roland Bliem, Oscar Gamba, Zdenek Jakub, Florian Brunbauer, Michael Schmid, Ulrike Diebold and Gareth S Parkinson  
“*A Multi-Technique Study of CO<sub>2</sub> Adsorption on Fe<sub>3</sub>O<sub>4</sub> Magnetite*”  
The Journal of Chemical Physics 146 014701 (2017)  
<http://dx.doi.org/10.1063/1.4973241>
44. Björn Arndt, Roland Bliem, Oscar Gamba, Jessi E.S. van der Hoeven, Heshmat Noei, Ulrike Diebold, Gareth S. Parkinson, Andreas Stierle  
“*Atomic structure and stability of magnetite Fe<sub>3</sub>O<sub>4</sub>(001): An X-ray view*”  
Surface Science 653 (2016), 76  
DOI: <http://dx.doi.org/10.1016/j.susc.2016.06.002>
43. Gareth S. Parkinson  
“*Iron Oxide Surfaces*”  
Surface Science Reports 71 (2016) 272  
DOI: [10.1016/j.surfrep.2016.02.001](http://dx.doi.org/10.1016/j.surfrep.2016.02.001)
42. Oscar Gamba, Jan Hulva, Jiri Pavelec, Roland Bliem, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
“*The role of surface defects in the adsorption of methanol on Fe<sub>3</sub>O<sub>4</sub>(001)*”  
Topics In Catalysis special issue – “Surface Chemistry of Well-Characterized Metal Oxides”  
DOI: <http://dx.doi.org/10.1007/s11244-016-0713-9>
41. 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, (2016) 8921  
DOI: <http://dx.doi.org/10.1073/pnas.1605649113>
40. Laura Martín-García, Arantzazu Mascaraque, Beatriz Martínez Pabon, Roland Bliem, Gareth S. Parkinson, Gong Chen, Andreas K. Schmid, and Juan de la Figuera  
“*Spin-reorientation transition of magnetite (001)*”  
Physical Review B 93 (2016) 134419  
DOI: <http://dx.doi.org/10.1103/PhysRevB.93.134419>
39. Gareth S. Parkinson, Peter Lackner, Oscar Gamba, Sebastian Maaß, Stefan Gerhold, Michele Riva, Roland Bliem, Ulrike Diebold and Michael Schmid  
“*Fe<sub>3</sub>O<sub>4</sub>(110)-(1×3) Revisited: Periodic (111) Nano-Facets*”  
Surface Science 649, 120-123 (2016)  
DOI: <http://dx.doi.org/10.1016/j.susc.2016.02.020>



38. Raquel Gargallo-Caballero, Laura Martín-García, Adrian Quesada, Cecilia Granados-Miralles, Michael Foerster, Lucia Aballe, Roland Bliem, Gareth Parkinson, Peter Blaha, José Marco, and Juan de la Figuera  
*“Co on Fe<sub>3</sub>O<sub>4</sub>(001): towards precise control of surface properties”*  
 The Journal of chemical physics 144 (9), 094704 (2016)  
 DOI: <http://dx.doi.org/10.1063/1.4942662>
37. Daniel Halwidl, Bernhard Stöger, Wernfried Mayr-Schmölzer, Jiri Pavelec, David Fobes, Jin Peng, Zhiqiang Mao, Gareth S Parkinson, Michael Schmid, Florian Mittendorfer, Josef Redinger, Ulrike Diebold  
*“Adsorption of water at the SrO surface of ruthenates”*  
 Nature Materials 15, 450–455 (2016)  
 DOI: <http://dx.doi.org/10.1038/nmat4512>
36. 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)  
 DOI: <http://dx.doi.org/10.1002/anie.201507368>
35. Martin Setvin, Maria Buchholz, Weiyi Hou, Cui Zhang, Bernhard Stöger, Jan Hulva, Thomas Simschitz, Xiao Shi, Jiri Pavelec, Gareth S Parkinson, Mingchun Xu, Yuemin Wang, Michael Schmid, Christof Wöll, Annabella Selloni, Ulrike Diebold  
*A Multitechnique Study of CO Adsorption on the TiO<sub>2</sub> Anatase (101) Surface*  
 The Journal of Physical Chemistry C 119 (36), 21044-21052  
 DOI: <http://dx.doi.org/10.1021/acs.jpcc.5b07999>
34. R. Bliem, J. Pavelec, O. Gamba, E. McDermott, Z. Wang, S. Gerhold, M. Wagner, J. Osiecki, K. Schulte, M. Schmid, P. Blaha, U. Diebold, G.S. Parkinson,  
*“Adsorption and Incorporation of Transition Metals at the Magnetite Fe<sub>3</sub>O<sub>4</sub>(001) Surface”*  
 Physical Review B 92 (2015) 075440  
 DOI: <http://dx.doi.org/10.1103/PhysRevB.92.075440>
33. 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.  
 DOI: <http://dx.doi.org/10.1126/science.1260556>
32. Oscar Gamba, Heshmat Noei, Roland Bliem, Michael Schmid, Ulrike Diebold, Andreas Stierle, Gareth S. Parkinson,  
*“Adsorption of Formic Acid and Methanol on the Fe<sub>3</sub>O<sub>4</sub> (001) Surface.”*  
 The Journal of Physical Chemistry C 119 (2015) 20459-20465  
 DOI: <http://dx.doi.org/10.1021/acs.jpcc.5b05560>
31. Bernhard Stöger, Marcel Hieckel, Florian Mittendorfer, Zhiming Wang, Michael Schmid, Gareth S. Parkinson, David Fobes, Jin Peng, J.E. Ortmann, Andreas Limbeck, Zhiqiang Mao, Josef Redinger, Ulrike Diebold  
*“Point Defects at Cleaved Sr<sub>n+1</sub>Ru<sub>n</sub>O<sub>3n+1</sub> (001) Surfaces”*  
 Phys. Rev. B 90, 165438 (2014)  
 DOI: <http://dx.doi.org/10.1103/PhysRevB.90.165438>
30. James J. Spivey, Katla Sai Krishna, Challa S.S.R. Kumar, Kerry M. Dooley, John C. Flake, Louis H. Haber, Ye Xu, Michael J. Janik, Susan B. Sinnott, Yu-Ting Cheng, Tao Liang, David S. Sholl, Thomas A. Manz, Ulrike Diebold, Gareth S. Parkinson, David A. Bruce, and Petra de Jongh

- “Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design.”*  
J. Phys. Chem. C 118, 20043 (2014)  
DOI: <http://dx.doi.org/10.1021/jp502556u>
29. R. Bliem, R. Kosak, L. Perneczky, Z. Novotny, Z. Mao, M. Schmid, P. Blaha, U. Diebold, G.S. Parkinson  
*“Cluster Nucleation and Growth from a Highly Supersaturated Adatom Phase: Ag/Fe<sub>3</sub>O<sub>4</sub>(001)”*  
ACS Nano 8, 7531-7537 (2014)  
DOI: <http://dx.doi.org/10.1021/nn502895s>
28. M. Setvin, X. Hao, B. Daniel, J. Pavelec, Z. Novotny, G.S. Parkinson, M. Schmid, G. Kresse, C. Franchini, and U. Diebold.  
*“Charge Trapping at the Step Edges of TiO<sub>2</sub> Anatase (101)”*  
Angew. Chem. Int. Edit. 53, 4714 (2014)  
DOI: <http://dx.doi.org/10.1002/anie.201309796>
27. J. de la Figuera, Z. Novotny, M. Setvin, T. Liu, Z. Mao, G. Chen, M. Schmid, U. Diebold, A.K. Schmid, G.S. Parkinson,  
*“Real-space imaging of the Verwey transition at the (100) surface of magnetite”*,  
Phys. Rev. B (Rapid Comm.), 88, 161410 (2013)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.88.161410>
26. 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”*  
Nat. Mater., 12, 724 (2013)  
DOI: <http://dx.doi.org/10.1038/nmat3667>
25. Z. Novotny, N. Mulakaluri, Z. Edes, M. Schmid, R. Pentcheva, U. Diebold, and G. S. Parkinson.  
*“Probing the surface phase diagram of Fe<sub>3</sub>O<sub>4</sub>(001) towards the Fe rich limit: Evidence for progressive reduction of the surface”*  
Phys. Rev. B 87, 195410 (2013)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.87.195410>
24. A.J. Window, A. Hentz, D.C. Sheppard, G.S. Parkinson, D.P. Woodruff, W. Unterberger, M.V. Ganduglia-Pirovano, J. Sauer.  
*“The structure of epitaxial V<sub>2</sub>O<sub>3</sub> films and their surfaces: a medium energy ion scattering study”*  
Surf. Sci. 606, 1716–1727 (2012)  
DOI: <http://dx.doi.org/10.1016/j.susc.2012.07.015>
23. 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)  
DOI: <http://dx.doi.org/10.1103/PhysRevLett.108.216103>
22. P. Jacobson, B. Stöger, A. Garhofer, G.S. Parkinson, M. Schmid, R. Caudillo, F. Mittendorfer, J. Redinger, U. Diebold,  
*“Nickel Carbide as a Source of Grain Rotation in Epitaxial Graphene”*  
ACS Nano 6, 3564-3572 (2012)  
DOI: <http://dx.doi.org/10.1021/nn300625y>
21. G. S. Parkinson, T. A. Manz, Z. Novotny, P. T. Sprunger, R. L. Kurtz, M. Schmid, D. S. Sholl, and U. Diebold,  
*“Anti-phase domain boundaries at the Fe<sub>3</sub>O<sub>4</sub>(001) surface”*



- Phys. Rev. B 85, 195450 (2012)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.85.195450>
20. P. Jacobson, B. Stoger, A. Garhofer, G. S. Parkinson, M. Schmid, R. Caudillo, F. Mittendorfer, J. Redinger, and U. Diebold.  
“Disorder and Defect Healing in Graphene on Ni(111)”  
J. Phys. Chem. Lett. 3, 136 (2012)  
DOI: <http://dx.doi.org/10.1021/jz2015007>
19. A. J. Window, A. Hentz, D. C. Sheppard, G. S. Parkinson, H. Niehus, D. Ahlbehrendt, T. C. Q. Noakes, P. Bailey, and D. P. Woodruff.  
“V<sub>2</sub>O<sub>3</sub>(0001) Surface Termination: Phase Equilibrium”  
Phys. Rev. Lett. 107, 016105 (2011)  
DOI: <http://dx.doi.org/10.1103/PhysRevLett.107.016105>
18. G.S. Parkinson, Z. Novotný, P. Jacobson, M. Schmid and U. Diebold.  
“Room Temperature Water Splitting at the Surface of Magnetite”  
J. Am. Chem. Soc. 133, 12650-12655, (2011)  
DOI: <http://dx.doi.org/10.1021/ja203432e>
17. G.S. Parkinson, Z. Novotný, P. Jacobson, M. Schmid and U. Diebold,  
“A metastable Fe(A) termination at the Fe<sub>3</sub>O<sub>4</sub>(001) surface”  
Surf. Sci. Lett., 605, L42, (2011)  
DOI: <http://dx.doi.org/10.1016/j.susc.2011.05.018>
16. G.S. Parkinson, N. Mulakaluri, Y. Losovyj, P. Jacobson, R. Pentcheva, U. Diebold.  
“Semiconductor-half metal transition at the Fe<sub>3</sub>O<sub>4</sub>(001) surface upon hydrogen adsorption”.  
Phys. Rev. B 82, 125413 (2010)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.82.125413>
15. G.S. Parkinson, Z. Dohnalek, R.S. Smith, B.D. Kay.  
“Reactivity of Fe<sup>0</sup> Atoms with Mixed CCl<sub>4</sub> and D<sub>2</sub>O Films over FeO(111)”  
J. Phys. Chem. C, 114, 17136-17141 (2010)  
DOI: <http://dx.doi.org/10.1021/jp103896k>
14. A.J. Window, A. Hentz, D.C. Sheppard, G.S. Parkinson, D.P. Woodruff, T.C.Q. Noakes, P. Bailey,  
“Silver sulphide growth on Ag(111): A medium energy ion scattering study”.  
Surf. Sci., 604, 1254 (2010)  
DOI: <http://dx.doi.org/10.1016/j.susc.2010.04.009>
13. D.C. Sheppard, G.S. Parkinson, A. Hentz, A.J. Window, P.D. Quinn, D.P. Woodruff, P. Bailey, T.C.Q. Noakes,  
“Medium energy ion scattering investigation of methylthiolate-induced modification of the Au(111) surface”  
Surf. Sci., 605, 138 (2011)  
DOI: <http://dx.doi.org/10.1016/j.susc.2010.10.011>
12. D.C. Sheppard, G.S. Parkinson, A. Hentz, P.D. Quinn, M.A. Muñoz-Márquez, D.P. Woodruff, P. Bailey, T.C.Q. Noakes,  
“Surface relaxation in Cu(410)-O: A medium energy ion scattering study”  
Surf. Sci., 604,788 (2010)  
DOI: <http://dx.doi.org/10.1016/j.susc.2010.02.001>
11. Y.K. Kim, Z.R. Zhang, G.S. Parkinson, S.C. Li, B.D. Kay, Z. Dohnalek,  
“Reactivity of FeO(111)/Pt(111) with Alcohols”,

- J. Phys. Chem. C 113, 20020-20028 (2009)  
DOI: <http://dx.doi.org/10.1021/jp907844j>
10. G.S. Parkinson, Z. Dohnalek, R.S. Smith, B.D. Kay,  
“Reactivity of  $C_2Cl_6$  and  $C_2Cl_4$  Multilayers with  $Fe^0$  Atoms over  $FeO(111)$ ”,  
J. Phys. Chem. C 113, 10233-10241 (2009)  
DOI: <http://dx.doi.org/10.1021/jp901040f>
  9. G.S. Parkinson, Y.K. Kim, Z. Dohnalek, R.S. Smith, B.D. Kay,  
“Reactivity of  $Fe^0$  Atoms and Clusters with  $D_2O$  over  $FeO(111)$ ”,  
J. Phys. Chem. C 113, 4960 (2009)  
DOI: <http://dx.doi.org/10.1021/jp810143y>
  8. A. Hentz, G.S. Parkinson, A. Window, D.P. Woodruff, P.L. Grande, G. Schiwietz, P. Bailey,  
T.C.Q. Noakes,  
“Direct observation and theory of trajectory-dependent electronic energy losses in medium-  
energy ion scattering”  
Phys. Rev. Lett. 102, 096103 (2009)  
DOI: <http://dx.doi.org/10.1103/PhysRevLett.102.096103>
  7. G.S. Parkinson, Z. Dohnalek, R.S. Smith, B.D. Kay,  
“Reactivity of  $Fe^0$  Atoms, Clusters, and Nanoparticles with  $CCl_4$  Multilayers on  $FeO(111)$ ”  
J. Phys. Chem. C 113, 5, 1818-1829 (2009)  
DOI: <http://dx.doi.org/10.1021/jp8076062>
  6. G.S. Parkinson, P.D. Quinn, D.P. Woodruff, P. Bailey, T.C.Q. Noakes,  
“Methylthiolate-induced reconstruction of  $Ag(1\ 1\ 1)$ : A medium energy ion scattering study”  
Surf. Sci 601, 50-57 (2007)  
DOI: <http://dx.doi.org/10.1016/j.susc.2006.09.007>
  5. A. Hentz, G.S. Parkinson, P.D. Quinn, M.A. Muñoz-Marquez, D.P. Woodruff, P.L. Grande, G.  
Schiwietz, P. Bailey, T.C.Q. Noakes,  
“Inelastic energy loss in 100-keV  $H^+$  scattering from single atoms: Theory and experiment for  
 $K$ ,  $Rb$ , and  $Cs$ ”  
Phys. Rev. B 74, 125408 (2006)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.74.125408>
  4. G.S. Parkinson, M.A. Muñoz-Márquez, P.D. Quinn, M.J. Gladys, R.E. Tanner, D.P. Woodruff,  
P. Bailey, T.C.Q. Noakes,  
“Medium-energy ion-scattering study of the structure of clean  $TiO_2(110)-(1\times 1)$ ”  
Phys. Rev. B 73, 245409 (2006)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.73.245409>
  3. G.S. Parkinson, M.A. Muñoz-Márquez, P.D. Quinn, M.J. Gladys, D.P. Woodruff, P. Bailey,  
T.C.Q. Noakes,  
“The methanethiolate-induced pseudo- $(1\ 0\ 0)$  reconstruction of  $Cu(1\ 1\ 1)$ : A medium energy  
ion scattering structure study”  
Surf. Sci 598, 209-217 (2005)  
DOI: <http://dx.doi.org/10.1016/j.susc.2005.08.038>
  2. M.A. Muñoz-Márquez, G.S. Parkinson, D.P. Woodruff, A. Hentz, P.L. Grande, G. Schiwietz,  
T.J. Wood, C. Bonet, S.P. Tear, P. Bailey, and T.C.Q. Noakes,  
“Energy loss in medium-energy ion scattering: A combined theoretical and experimental study  
of the model system  $Y$  on  $Si(111)$ ”  
Phys. Rev. B 72, 075415 (2005)  
DOI: <http://dx.doi.org/10.1103/PhysRevB.72.075415>

1. M.A. Munoz-Marquez, G.S. Parkinson, P.D. Quinn, M.J. Gladys, R.E. Tanner, D.P. Woodruff,  
“*N*-induced pseudo-(1 0 0) reconstruction of Cu(1 1 1): One layer or more?”  
Surf. Sci. 582, 97-109 (2005)  
DOI: <http://dx.doi.org/10.1016/j.susc.2005.03.008>

**Other Publications –**

2018 - Atomic Scale Insights Into Single-Atom Catalysis

Invited Article for ViP (Vacuum in Research and Practise), the members’ magazine of the German Vacuum Society

<https://doi.org/10.1002/vipr.201800695>

2013 - [Experiment & Theory: The Perfect Marriage](#) – Editorial article for the Energy Frontier Research Centre Newsletter