Prof. Dr. Reinhard J. Maurer

Professor of
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Academic Career

11/2022 – present	**Professor of Computational Physics** (joint appointment), University of Warwick, UK
08/2022 – present	**Professor of Computational Chemistry**, University of Warwick, UK
08/2020 – 07/2022	**Associate Professor of Computational Chemistry**, University of Warwick, UK
09/2017 – 07/2020	**Assistant Professor of Computational Chemistry**, University of Warwick, UK
11/2014 – 08/2017	**Postdoctoral Research Associate**, Department of Chemistry, Yale University, USA Supervisor: Prof. John C. Tully
03/2014 – 10/2014	**Postdoctoral Research Associate**, Department Chemie, TU Munich, Germany
10/2010 – 02/2014	**PhD in Theoretical Chemistry**, Department Chemie, TU Munich, Germany Supervisor: Prof. Karsten Reuter, defended on 27.01.2014 with *summa cum laude*
10/2005 – 07/2010	**Diploma in Chemistry**, Institut für Chemie, University of Graz, Austria

Fellowships and Awards

2024	Royal Society of Chemistry, Faraday early career prize: Marlow Prize
2022	ERC Starting Grant (€1,50 million)
2022	IOP Electronic Structure, Emerging Leader
2021	Andrew McCamley Teaching Award of the Department of Chemistry, U Warwick
2020	IOP Journal of Physics: Condensed Matter, Emerging Leader
2019	UKRI Future Leaders Fellowship (£1,15 million)
2018	Runner-up to the Psi-K Volker Heine Early Career Award of the Psi-K community and the German Physical Society (1 of 5 finalists), awarded for *"outstanding early career contributions to first principles methodology and electronic structure calculations"*
2018	IOP Journal of Physics: Condensed Matter, Emerging Leader
2016	Visiting Fellow at Institute of Pure and Applied Mathematics, UCLA, USA
2016	Strategy& Presidential Award of the Technical University Munich *1 price/year across all disciplines and faculties for* *"outstanding research and teaching accomplishments in the area of nanofunctionalized materials and the translation of deep chemical understanding into modern computing algorithms"*
2014	Teaching fellowship of the German academic exchange service (DAAD)
2007 – 2010	3 times recipient of the merit scholarship of faculty of science, University of Graz
2007 – 2010	3 times recipient of the merit scholarship of the Austrian federal state of Styria

Publication Track Record

A total of **92 publications** in peer-reviewed journals, including:

Angewandte Chem Int. Ed. (x2)	Nano Letters and ACS Nano (x5)	Nature Commun (x3)
Physical Review Letters (x6)	J. Phys. Chem. Lett. (x4)	Chem. Sci. (x2)

- >4000 citations, H-index = 32 (Google Scholar, June 27th, 2024)

For details see publication list below

Funding Record

Total research income as independent researcher beyond £5.0 million

2023	UKRI FLF renewal (£567k), MSCA PostDoc Fellowship (£187k), Co-I on EPSRC HPC-CONEXS grant (£372k), MSCA Staff Exchange grant (£336k), Leverhulme Trust (£339k)
2022	ERC Starting Grant (£1,25 million), Warwick Research Development Fund (£25k)
2021	2x EPSRC/eCSE ARCHER2-funded PostDoc (£85k) (1 as PI, 1 as Co-I)
2020	1x Industrial-cofunded PhD studentship (£51k), EPSRC/eCSE ARCHER2-funded PostDoc (£81k), Industrial-funded PostDoc (£22k), Host of FWF-funded PostDoc Fellow (£73k), Host of DFG-funded PostDoc Fellow (£52k)
2019	UKRI Future Leaders Fellowship: incl. 2x PostDoc (£1,15 million), Leverhulme Trust Project Grant: 2x PhD studentships (£150k), EPSRC-funded PostDoc (£34k), Host of EC-MSCA-COFUND PostDoc Fellow (£96k), 1x Industrial-cofunded PhD studentship (£51k), 1x EPSRC-funded PhD studentship (£77k)
2018	U Warwick-funded PostDoc (£25k), 4x EPSRC-funded PhD studentship (£75k each)
2011-2023	Numerous HPC time proposals funded via, PRACE(DECI), MCC-HEC (EPSRC), UKRI, Bavarian Academy of Science, Helmholtz Research Society, totalling an average 20M CPUh per year.

Presentation Track Record

Summary: **42 invited talks at international conferences, 34 invited talks at department/university seminars**, 13 contributed conference talks, 12 poster contributions, with highlights including:

2023	Gordon Research Conference on Dynamics at Surfaces, Newport, USA
2021	CECAM Workshop “Challenges in Reaction Dynamics of Gas-Surface Interactions and Methodological Advances in Dissipative and Non-Adiabatic Processes”, Toulouse, France
2020	ACS Fall Meeting Symposium "From Bench to Market: Leveraging AI & Advanced Computational Methods to Solve Hard Problems", San Francisco, USA
2018	International Materials Research Conference (IMRC), Cancun, Mexico
2017	Spring meeting of the Condensed Matter Section of the German Physical Society (DPG)

For details see attached presentation list

Supervision Record

2017 – present	**University of Warwick**, Department of Chemistry, UK 13 Postdoctoral Researchers (6 at present) 18 PhD students (10 at present, 8 graduated) 8 MSc students (Chemistry and Physics) and 5 Undergraduate researchers
2015 – 2016	**Yale University**, Department of Chemistry, USA 1 PhD student + 1 visiting MSc student
2010 – 2015	**Technical University Munich**, Department Chemie, Germany 5 Masters students + 3 Bachelors students

Academic Service

2020 – present **Editorial Board Member** for

- *Communications Materials* Nature journal
- *SciPost Chemistry* journal

2018 – present **Examiner** at 8 PhD defences:
TU Graz (Austria), 2x U Vienna (Austria), U of Leiden (Netherlands), U Cardiff (UK), 2x U Warwick (UK), Queen’s University Belfast (UK)

2016 – present	**Grant review activity** for EPSRC, UK Research and Innovation (UKRI), German research funding agency (DFG), Dutch funding agency (NWO), ERC CoG, AdG, SyG Grants, and EC-MSCA programmes, Royal Society URF programme, US DoE, Israel Science Foundation
2012 – present	**Peer review activity** for journals published by Institute of Physics, RSC, ACS, APS, Nature Group Examples: JACS, Nature Communications, Phys. Rev. Lett., J. Phys. Chem. Lett., Phys. Rev B, J. Chem. Phys., Machine Learning: Science and Technology (IOP)

Organization of Scientific Conferences

10/2024	Organisation of Conference "Ultrafast phenomena and light-matter interaction in quantum materials (UltraLight)", Zadar, Croatia
05/2024	Organisation of FHI-aims UK Meeting 2024, University of Warwick
03/2024	Organisation of Focus Session on "Advances in Ab-Initio Electronic Structure Theory of Time-Dependent and Non-Equilibrium Phenomena" at the German Physical Society (DPG) Spring Meeting
09/2023	Organisation of Machine Learning for Atomistic Modelling Autumn School 2023, Daresbury Laboratory, UK
03/2023	Machine Learning in Materials Research 1-day networking event for UK researchers, Abingdon, outcome documented as white paper and circulated to policy makers
07/2022	Organisation of CECAM Flagship Workshop "Light-matter interaction and ultrafast nonequilibrium dynamics in plasmonic materials", University of Warwick UK
02/2022	Organisation of international workshop "Dynamics, Quantum Effects, and Machine Learning in Materials Science and Computational Chemistry (DQML 2022)"
03/2020	Organisation of Focus Session on "Electron-Driven Processes: Atomic-scale Insights from Theory and Experiment" at the German Physical Society (DPG) Spring Meeting [COVID cancelled]
04/2019	Organisation of international conference on Computational Molecular Science (CMS2019) at University of Warwick, 165 participants. Biggest UK computational chemistry conference
02/2015	Organisation of international workshop at Rudolfshuette, Austria on First-Principles-Based Multiscale Modelling in Materials, Energy, and Catalysis, 40 participants

Membership of Professional Societies

Since 2023	Board Member of European Conference on Surface Crystallography and Dynamics (ECSCD)
Since 2023	Elected Executive Member of the American Vacuum Society Surface Science Division
Since 2021	Elected Member of the RSC Faraday Community Council for Physical Chemistry
Since 2020	Member of the American Chemical Society (ACS)
Since 2019	Fellow of the Higher Education Academy (HEA) *HEA: UK Certification Agency for Teaching at Higher Education Institutions*
Since 2017	Member of the Royal Society of Chemistry (RSC)
Since 2010	Member of the German Physical Society (DPG)

Institutional Responsibilities (at U Warwick, UK)

2022 – present	Member of Equality, Diversity and Inclusion Committee, Department of Chemistry
2021 – present	Member of Faculty of Science IT Committee

2022 – 2023	Director of Graduate Studies, Department of Chemistry
2022 – 2023	Member of Department of Chemistry Executive Committee
2018 – 2020	Member of the Undergraduate Admissions Committee for Chemistry (Marketing coordination and co-organisation of Offer Holder Days)
2018 – present	Member of the HPC Midlands+ Strategic User Group
2018 – present	Member of the Advisory PhD Committee for >12 PhD students in Chemistry
2019 – 2021	Project lead in deploying a computational hardware/software infrastructure for Jupyter-notebook-based computational key skills undergraduate training in STEM

Major Collaborations

- Collaborations with leading research groups that provide complementary theoretical/computational expertise: Prof. Hua Guo (U New Mexico, US), Prof. Bin Jiang (USTC, China), Prof. Klaus-Robert Müller (TU Berlin, DE), Prof. Alexandre Tkatchenko (U. Luxembourg, LU), Prof. Christoph Ortner (UBC, Canada), Prof. James Kermode (U Warwick, UK), Prof. Michael Thoss (Freiburg, DE)
- Strong network of experimental collaborators in surface science and surface electro- and photochemistry: Prof. Giovanni Costantini, Prof. Phil Woodruff, Prof. Pat Unwin, and Prof. Julie Macpherson (U Warwick, UK), Dr. David Duncan (Diamond Light Source, UK), Dr. Christian Wagner and Prof. F. Stefan Tautz (Helmholtz Research Centre Jülich, DE), Prof. Michael Gottfried (U. Marburg, DE), Prof. Alec Wodtke (MPI Goettingen, DE)

List of Publications

[93] S. J. Hall, B. P. Klein, **R. J. Maurer**, "*Self-interaction error induces spurious charge transfer artefacts in core-level simulations of x-ray photoemission and absorption spectroscopy of metal-organic interfaces*", arXiv:2112.00876 (2023)

[92] G. Meng, J. Gardner, W. Dou, **R. J. Maurer**, B. Jiang, "*First-principles Nonadiabatic Dynamics of Molecules at Metal Surfaces with Vibrationally Coupled Electron Transfer*", Phys. Rev. Lett., in press, arXiv:2401.02316 (2024)

[91] W. G. Stark, C. v. d. Oord, I. Batatia, Y. Zhang, B. Jiang, G. Csanyi, **R. J. Maurer**, "*Benchmarking of machine learning interatomic potentials for reactive hydrogen dynamics at metal surfaces*", IOP Machine Learning: Science and Technology, in press, arXiv:2403.15334 (2024)

[90] J. Gilkes, M. Storr, **R. J. Maurer**, S. Habershon, "*Predicting Long Timescale Kinetics under Variable Experimental Conditions with Kinetica.jl*", J. Chem. Theory Comput., in press (2024)

[89] M. A. Stoodley, L. A. Rochford, T.-L. Lee, B. P. Klein, D. A. Duncan, **R. J. Maurer** "*Structure of Graphene Grown on Cu(111): X-Ray Standing Wave Measurement and Density Functional Theory Prediction*", Phys. Rev. Lett. **132**, 196201 (2024)

[88] R. Bolat, J. M. Guevara, P. Leinen, M. Knol, H. H. Arefi, M. Maiworm, R. Findeisen, R. Temirov, O. T. Hofmann, **R. J. Maurer**, F. S. Tautz, C. Wagner, "*Electrostatic potentials of atomic nanostructures at metal surfaces quantified by scanning quantum dot microscopy*", Nature Commun. **15**, 2259 (2024)

[87] **R. J. Maurer**, P. J. Jain, *"Hot Electrons in Catalysis"*, J. Phys. Chem. C **128**, 1863-1866 (2024), Preface to Virtual Special Issue on "Hot Electrons in Catalysis".

[86] B. P. Klein, M. A. Stoodley, D. B. Morgan, L. A. Rochford, L. B. S. Williams, P. T. P. Ryan, L. Sattler, S. M. Weber, G. Hilt, T. J. Liddy, T.-L. Lee, **R. J. Maurer**, D. A. Duncan, *"Probing the role of surface termination in the adsorption of azupyrene on copper"*, Nanoscale **16**, 5802-5812 (2024)

[85] W. G. Stark, J. Westermayr, O. A. Douglas-Gallardo, J. Gardner, S. Habershon, **R. J. Maurer**, "*Importance of equivariant features in machine-learning interatomic potentials for reactive chemistry at metal surfaces*", J. Phys. Chem. C **127**, 24168-24182 (2023)

[84] J. Hermann, M. Stöhr, S. Góger, S. Chaudhuri, B. Aradi, **R. J. Maurer**, A. Tkatchenko, "libMBD: A general-purpose package for scalable quantum many-body dispersion calculations", J. Chem. Phys. **159**, 174802 (2023)

[83] N. Hertl, **R. J. Maurer**, "*Energy transfer during hydrogen atom collisions with surfaces*", Trends in Chemistry **5**, 795-798 (2023)

[82] C. L. Box, W. G. Stark, **R. J. Maurer**, "*Ab initio calculation of electron-phonon linewidths and molecular dynamics with electronic friction at metal surfaces with numeric atom-centered orbitals*", IOP Electronic Structure **5**, 035005 (2023), Special Issue "Emerging Leaders 2021"

[81] S. Chaudhuri, A. J. Logsdail, **R. J. Maurer**, "*Stability of Single Metal Atoms on Defective and Doped Diamond Surfaces*", J. Phys. Chem C **127**, 16187-16203 (2023)

[80] J. Gardner, S. Habershon, **R. J. Maurer**, "*Assessing mixed quantum-classical molecular dynamics methods for nonadiabatic dynamics of molecules on metal surfaces*", J. Phys. Chem. C **127**, 15257-16270 (2023)

[79] P. V. Stishenko, T. W. Keal, S. M. Woodley, V. Blum, B. Hourahine, **R. J. Maurer**, A. J. Logsdail, "*Atomic Simulation Interface (ASI): application programming interface for electronic structure codes*", J. Open Source Software **8** (85), 5186 (2023)

[78] A. Baklanov, J. T. Kuchle, D. A. Duncan, P. T. P. Ryan, **R. J. Maurer**, M. Schwarz, E. C. Rascon, I. Piquero-Zulaica, H. T. Ngo, A. Riss, F. Allegretti, W. Auwärter, "*Zinc-Porphine on Coinage Metal Surfaces: Adsorption Configuration and Ligand-Induced Central Atom Displacement*", J. Phys. Chem. C **127**, 7501-7512 (2023)

[77] J. Gardner, D. Corken, S. M. Janke, S. Habershon, **R. J. Maurer**, *"Efficient implementation and performance analysis of the independent electron surface hopping method for dynamics at metal surfaces"*, J. Chem. Phys. **158**, 064101 (2023)

[76] J. Westermayr, J. Gilkes, R. Barrett, **R. J. Maurer**, "*High-throughput property-driven generative design of functional organic molecules",* Nature Comput. Sci. **3**, 139-148 (2023)

[75] B. Sohail, P. J. Blowey, L. A. Rochford, P. T. P. Ryan, D. A. Duncan, T.-L. Lee, P. Starrs, G. Costantini, D. P. Woodruff, **R. J. Maurer**, *"Donor-acceptor co-adsorption ratio controls structure and electronic properties of two-dimensional alkali-organic networks on Ag(100)",* J. Phys. Chem. C **127**, 2716-2727 (2023)

[74] S. J. Hall, B. Klein, **R. J. Maurer**, "*Characterizing Molecule-Metal Surface Chemistry with Ab-Initio Simulation of X-ray Absorption and Photoemission Spectra*", J. Phys. Chem. C **127**, 1870-1880 (2023) Special Issue "Early Career and Emerging Researchers in Physical Chemistry"

[73] B. P. Klein, M. A. Stoodley, M. Edmondson, L. A. Rochford, M. Walker, L. Sattler, S. M. Weber, G. Hilt, L. B. S. Williams, T.-L. Lee, A. Saywell, **R. J. Maurer**, D. A. Duncan, "*Using polycyclic aromatic hydrocarbons for graphene growth on Cu(111) under ultra-high vacuum*", Appl. Phys. Lett. **121**, 191603 (2022)

[72] Y. Zhang, C. L. Box, T. Schäfer, A. Kandratsenka, A. M. Wodtke, **R. J. Maurer**, B. Jiang, "*Stereodynamics of Adiabatic and Non-adiabatic Energy Transfer in a Molecule Surface Encounter*", Phys Chem. Chem. Phys.: PCCP **24**, 19753-19760 (2022)

[71] B. P. Klein, A. Ihle, S. R. Kachel, L. Ruppenthal, S. J. Hall, L. E. Sattler, S. M. Weber, J. Herritsch, A. Jaegermann, D. Ebeling, **R. J. Maurer**, G. Hilt, R. Tonner, A. Schirmeisen, J. M. Gottfried, "*Topological Stone-Wales Defect Enhances Bonding and Electronic Coupling at the Graphene/Metal Interface*", ACS Nano **16**, 11979-11987 (2022)

[70] L. Zhang, B. Onat, G. Dusson, G. Anand, **R. J. Maurer**, C. Ortner, J. R. Kermode, "*Equivariant analytical mapping of first principles Hamiltonians to accurate and transferable materials models*", npj Comput. Mater. Sci. **8**, 158 (2022)

[69] J. Westermayr, S. Chaudhuri, A. Jeindl, O. T. Hofmann, **R. J. Maurer**, "*Long-range dispersion-inclusive machine learning potentials for structure search and optimization of hybrid organic-inorganic interfaces*", RSC Digital Discovery **1**, 463-475 (2022)

[68] Y. Litman, E. S. Pos, C. L. Box, R. Martinazzo**, R. J. Maurer**, M. Rossi, "*Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory II: Benchmarks and Applications*", J. Chem. Phys. **156**, 194107 (2022)

[67] Y. Litman, E. S. Pos, C. L. Box, R. Martinazzo, **R. J. Maurer**, M. Rossi, "*Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory I: Theory*", J. Chem. Phys. **156**, 194106 (2022)

[66] J. Gardner, O. A. Douglas-Gallardo, W. G. Stark, J. Westermayr, S. M. Janke, S. Habershon, **R. J. Maurer**, "*NQCDynamics.jl: A Julia Package for Nonadiabatic Quantum Classical Molecular Dynamics in the Condensed Phase*", J. Chem. Phys. **156**, 174801 (2022)

[65] P. J. Mousley, L. A. Rochford, P. T. P. Ryan, P. J. Blowey, J. Lawrence, D. A. Duncan, H. Hussain, B. Sohail, T.-L. Lee, G. R. Bell, G. Costantini, **R. J. Maurer**, D. P. Woodruff, "*Direct experimental evidence for substrate adatom incorporation into a molecular overlayer*", J. Phys. Chem. C **126**, 6880-6891 (2022)

[64] H. Arefi, D. Corken, F. S. Tautz, **R. J. Maurer**, C. Wagner, „*Design principles for metastable standing molecules*", J. Phys. Chem. C **126**, 6880-6891 (2022)

[63] P. Rhyan, P. J. Blowey, B. S. Sohail, L. A. Rochford, D. A. Duncan, T.-L. Lee, P. Starrs, G. Costantini, **R. J. Maurer**, D. P. Woodruff, "*Thermodynamic Driving Forces for Substrate Atom Extraction by Adsorption of Strong Electron Acceptor Molecules*", J. Phys. Chem. C **126**, 6082-6090 (2022)

[62] M. R. Lea, V. G. Stavros, **R. J. Maurer**, "*Effect of electron donating/withdrawing groups on molecular photoswitching of functionalized hemithioindigo derivatives: a computational multireference study*", ChemPhotoChem **6**, e202100290 (2022)

[61] H. Kulik et al. "*Roadmap on Machine Learning in Electronic Structure*", IOP Electronic Structure (2022), DOI: 10.1088/2516-1075/ac572f

[60] S. Chaudhuri, S. J. Hall, B. P. Klein, M. Walker, A. J. Logsdail, J. V. Macpherson, **R. J. Maurer**, "*Coexistence of carbonyl and ether groups on oxygen-terminated (110)-oriented diamond surfaces*", Communications Materials **3**, 6 (2022)

[59] J. M. Kahk, G. S. Michelitsch**, R. J. Maurer**, K. Reuter, J. Lischner, "*Core Electron Binding Energies in Solids from Periodic All-Electron Δ-Self-Consistent-Field Calculations*", J. Phys. Chem. Lett. **12**, 9353-9359 (2021)

[58] D.-Q. Liu, M. Kang, D. Perry, C.-H. Chen, G. West, X. Xia, Z. P. L. Laker, N. R. Wilson, M. Melander, **R. J. Maurer**, P. R. Unwin, *"Adiabatic versus Non-Adiabatic Electron Transfer at 2D Electrode Materials",* Nature Commun. **12**, 7110 (2021)

[57] M. Knol, H. H. Arefi, D. Corken, J. Gardner, F. S. Tautz, **R. J. Maurer**, C. Wagner, "*The stabilization potential of a standing molecule*", Science Advances **7**, eabj9751 (2021)

[56] O. A. Douglas-Gallardo, C. L. Box, **R. J. Maurer**, *"Plasmonic enhancement of molecular hydrogen dissociation on metallic magnesium nanoclusters"*, Nanoscale **13**, 11058-11068 (2021) Back Cover of Journal Issue

[55] J. Westermayr, **R. J. Maurer**, *"Physically inspired deep learning of molecular excitations and photoemission spectra"*, Chem. Sci. **12**, 10755-10764 (2021)

[54] J. Westermayr, M. Gastegger, K. T. Schütt, **R. J. Maurer**, *"Perspective on integrating machine learning into computational chemistry and materials science"*, J. Chem. Phys. **154**, 230903 (2021), Invited Perspective

[53] B. P. Klein, L. Ruppenthal, S. J. Hall, L. E. Sattler, S. M. Weber, J. Herritsch, A. Jaegermann, **R. J. Maurer**, G. Hilt, J. M. Gottfried, "*Topology Effects in Molecular Organic Electronic Materials: Pyrene and Azupyrene*", PhysChemPhys **22**, 1065-1073 (2021)

[52] O. T. Hofmann, E. Zojer, L. Hörmann, A. Jeindl, **R. J. Maurer**, "*First-principles calculations of hybrid inorganic–organic interfaces: from state-of-the-art to best practice*", Phys. Chem. Chem. Phys. **23**, 8132-8180 (2021)

[51] B. Klein, S. J. Hall, **R. J. Maurer**, *"The Nuts and Bolts of Core-Hole Constrained Ab-Initio Simulation for K-shell X-Ray Photoemission and Adsorption Spectra",* J. Phys.: Condens. Matter **33**, 154405, Invited Article in Special Issue "Emerging Leaders 2020" (2021)

[50] C. L. Box, Y. Zhang, R. Yin, B. Jiang, **R. J. Maurer**, *"Determining he Effect of Hot Electron Dissipation on Molecular Scattering Experiments at Metal Surfaces*", JACS Au **1**, 164-173 (2021)

[49] M. Gastegger, A. McSloy, M. Luya, K. T. Schütt, **R. J. Maurer**, *"A deep neural network for molecular wave functions in quasi-atomic minimal basis representation"*, J. Chem. Phys. **153**, 044123 (2020).

[48] P. J. Blowey, B. Sohail, L. A. Rochford, T. Lafosse, D. A. Duncan, D. Warr, T.-L. Lee, G. Costantini, **R. J. Maurer**, D. P. Woodruff, *"Alkali doping leads to salt formation in a two-dimensional metal-organic framework: K and TCNQ on Ag(111)"*, ACS Nano **14**, 7475–7483 (2020).

[47] B. Hourahine, B. Aradi, V. Blum, F. Bonafé, A. Buccheri, C. Camacho, C. Cevallos, M. Y. Deshaye, T. Dumitrica, A. Dominguez, S. Ehlert, M. Elstner, T. van der Heide, J. Hermann, S. Irle, J. J. Kranz, C. Köhler, T. Kowalczyk, T. Kubar, I. S. lee, V. Lutsker, **R. J. Maurer**, S. K. Min, I. Mitchell, C. Negre, T. A. Niehaus, A. M. N. Niklasson, A. J. Page, A. Peccia, G. Penazzi, M. P. Persson, J. Řezáč, C. G. Sánchez, M. Sternberg, M. Stöhr, F. Stuckenberg, A. Tkatchenko, V. W.-Z. Yu, and T. Frauenheim, *"DFTB+, a software package for efficient approximate density functional theory based atomistic simulations"*, J. Chem. Phys. **152**, 124101 (2020).

[46] B. P. Klein, S. E. Harman, L. Ruppenthal, G. M. Ruehl, S. J. Hall, S. J. Carey, J. Herritsch, M. Schmid, **R. J. Maurer**, R. Tonner, C. T. Campbell, J. Michael Gottfried, *"Enhanced Bonding of Pentagon–Heptagon Defects in Graphene to Metal Surfaces: Insights from the Adsorption of Azulene and Naphthalene to Pt(111)"*, Chem. Mater. **32**, 1041-1053 (2020).

[45] Y. Zhang, **R. J. Maurer**, B. Jiang, *"Symmetry-Adapted High Dimensional Neural Network Representation of Electronic Friction Tensor of Adsorbates on Metals"*, J. Phys. Chem. C, **124**, 186-195 (2019).

[44] K. T. Schütt, M. Gastegger, A. Tkatchenko, K.-R. Müller, and **R. J. Maurer**, "*Unifying machine learning and quantum chemistry with a deep neural network for molecular wavefunctions*", Nature Commun. **10**, 5024 (2019).

[43] B. P. Klein, J. M. Morbec, M. Franke, K. K. Greulich, M. Sachs, S. Parhizkar, F. C. Bocquet, M. Schmid, S. J. Hall, **R. J. Maurer**, B. Meyer, R. Tonner, C. Kumpf, P. Kratzer, J. Michael Gottfried, *"Molecule–Metal Bond of Alternant versus Nonalternant Aromatic Systems on Coinage Metal Surfaces: Naphthalene versus Azulene on Ag(111) and Cu(111)"*, J. Phys. Chem. C, 123, 29219-29230 (2019).

[42] R. Guttmann, J. Hoja, C. Lechner, **R. J. Maurer**, and A. F. Sax, "*Adhesion, forces and the stability of interfaces*", Beilstein J. Org. Chem. **15**, 106–129 (2019).

[41] M. Cueto, **R. J. Maurer**, F. Al Taleb, M. Daniel, F. Martin, and C. Diaz, "*Performance of van der waals dft approaches for helium diffraction on metal surfaces*", J. Phys.: Condens. Matter **31**, 135901 (2019).

[40] B. Klein, N. Van der Heijden, S. Kachel, M. Franke, C. K. Krug, K. Greulich, L. Ruppenthal, P. Müller, P. Rosenow, S. Parhizkar, F. Bocquet, M. Schmid, W. Hieringer, **R. J. Maurer**, R. Tonner, C. Kumpf, I. Swart, and G. J. Michael, "*A molecular model system for pentagon-heptagon (5-7) defects in supported graphene*", Phys. Rev. X **9**, 011030 (2019).

[39] **R. J. Maurer**, Y. Zhang, H. Guo, and B. Jiang, "*Hot-electron effects during reactive scattering of H_2 from Ag(111): assessing the sensitivity to initial conditions, coupling magnitude, and electronic temperature*", Faraday Discussions on "Hot-electron science and microscopic processes in plasmonics and catalysis" **214**, pp. 105-121 (2019).

[38] Y. Zhang, **R. J. Maurer**, H. Guo, and B. Jiang, "*Hot-electron effects during reactive scattering of H_2 from Ag(111): the interplay between mode-specific electronic friction and the potential energy landscape*", Chem. Sci. **10**, 1089–1097 (2019).

[37] **R. J. Maurer**, C. Freysoldt, A. M. Reilly, J. G. Brandenburg, O. T. Hofmann, T. Björkman, S. Lebégue, and A. Tkatchenko, "*Advances in density-functional calculations for materials modeling*", Annu. Rev. Mater. Res., Invited Review **49**, 1-30 (2019).

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List of Presentations

Only first-author contributions are listed.

List of Invited Conference Talks

[42] "X-ray spectroscopic signatures of chemical bonding and dynamics at metal-organic interfaces", presented at the Recent Advances in Computer-aided X-ray Spectroscopy CECAM workshop, Helsinki, Finland, 06/17-20/2024

[41] "Machine-learning-accelerated nonadiabatic dynamics at surfaces", presented at Machine Learning in Chemical and Materials Sciences 2024, virtual conference, 05/20-23/2024

[40] "*Machine learning prediction of electronic structure for high-throughput inverse design of functional organic materials*", presented at the Materials Research Society spring meeting, Seattle, USA, 04/24/2024

[39] "*Simulation of light- and electron-driven chemistry at surfaces and plasmonic nanoparticles*", presented at the Max Planck research conference (MPINAT), Castle Ringberg, Germany, 12/20/2023

[38] "*Machine learning of electronic structure for quantum dynamics and molecular design*", presented at the International Symposium on Machine Learning in Quantum Chemistry, Uppsala, Sweden, 12/01/2023
[37] "*First principles electronic friction theory to simulate quantum dynamics at surfaces*", presented at the Machine Learning and Simulation of Stochastic Dynamics with applications in materials science, University of Birmingham, UK, 09/22/2023
[36] **"***Ab Initio Simulation of Light- and Electron-Driven Chemistry at Surfaces and Plasmonic Nanoparticles*", presented at the Gordon Research Conference Dynamics at Surfaces 2023, Newport, RI, USA, 07/25/2023.
[35] "*High-throughput property-driven generative design of functional organic molecules*", presented at the International Conference on Chemical Bonding, Kauai, HI, USA, 07/22/2023
[34] "*High-throughput property-driven generative design of functional organic molecules*" presented at the Machine Learning in Materials Design and Discovery Workshop, University of Liverpool, 06/22/2023
[33] "*Dynamic charge-transfer at functional metal-organic interfaces: What is it and how can we control it?*", 747. WE Hereaus Seminar on "Molecular Functionality at Surfaces: Self-Assembly, Manipulation, Reactivity and the Role of Decoupling", Bad Honnef, Germany, 11/16/2022
[32] "*Machine learning of electronic structure for quantum dynamics and molecular design*", TSRC Telluride Machine Learning and Informatics for Chemistry and Materials Workshop, Colorado, USA, 10/06/2022
[31] "*Machine learning of electronic structure for dynamics at surfaces*", MLQC4Dyn Workshop "Machine Learning for Quantum Molecular Dynamics", Paris, France, 09/14/2022
[30] "*Deep learning surrogates of electronic structure for dynamics and molecular design*", Summer School for Machine Learning of Materials Hard and Soft, Erwin Schrödinger Institute of the University of Vienna, Vienna, Austria, 07/15/2022
[29] "*Hot electron energy dissipation in chemical reactions at metal surfaces*", Lorentz Center Workshop on Energy Dissipation at Interfaces: From Catalysis to Astrochemistry 2022, Leiden, The Netherlands, 05/16-05/20/2022
[28] "*Simulation of X-ray photoemission and absorption of metal-organic interfaces: Spectroscopic signatures of chemical bonding and dynamics*", CONEXS conference, Newcastle, UK, 03/30-04/1/2022
[27] "*Physically-inspired deep learning of electronic structure for the design of tailormade functional molecules*", AI4SD conference on Artificial Intelligence for Scientific Discovery, Southampton, UK, 03/01-03/03/2022
[26] "*Quantifying the limits of ab initio electronic friction theory*", CECAM workshop on "CHALLENGES IN REACTION DYNAMICS OF GAS--SURFACE INTERACTIONS AND METHODOLOGICAL ADVANCES IN DISSIPATIVE AND NON-ADIABATIC PROCESSES", Toulouse, France, 09/27-09/30/2021
[25] *"NO scattering on gold is still a challenge for nonadiabatic dynamics simulations",* TSRC Telluride Quantum Effects in Condensed-Phase Systems Workshop, Telluride, Colorado, USA, 06/30/2021
[24] *"Unifying Machine Learning and Quantum Chemistry: From Deep Learning of Wave Functions to ML/QM-hybrid Methods",* AI3SD (EPSRC-funded UK research network) virtual winter seminar, 02/24/2021
[23] "*Deep learning of local orbital Hamiltonians in minimal basis representation*", presented at the virtual DFTB-ML 2020 workshop (organized by U Bremen), 07/10/2020.
[22] *"Machine Learning Augmented Quantum Chemistry: From Deep Learning of Wave Functions to ML/QM-Tandem methods."* presented at the virtual ACS Fall Meeting, San Francisco, USA, 08/16-20/2020.
[21] "A deep neural network to represent molecular wave functions" presented at the virtual MACSIM 2020 workshop, 06/29 – 07/02/2020.
[20] "*Machine Learning is the oil that eases (electronic) friction: Dynamics at Surfaces with FHI-aims*" presented at the "FHI-aims Developers' and Users' Meeting", Humboldt University Berlin, Germany, 06/24/2020.
[19] *"Deep Learning Enhanced Quantum Chemistry: Pushing the Limits of Materials Discovery"*, presented at the "Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery (AI3SD) Network+ conference", Winchester, United Kingdom, 11/18/2019.

[18] "*Ab-initio simulation methods to study coupled electron-nuclear dynamics at surfaces*", presented at the Summer School on "Non-Equilibrium Dynamics of Condensed Matter in the Time Domain", Bad Honnef, Germany, 08/20/2019.
[17] **"***Ab initio simulation of hot-electron mediated chemistry at metal surfaces"*, TSRC Telluride Quantum Effects in Condensed-Phase Systems Workshop, Telluride, Colorado, USA, 07/30/2019
[16] "*Deep Tensor Neural Network Representation of the Electronic Structure of Molecules*", presented at the 2nd IPAM Reunion Workshop on "Understanding Many-Particle Systems with Machine Learning", Lake Arrowhead, USA, 06/14/2019.
[15] "*A first-principles perspective on the electronic and spectroscopic signatures of charge transfer at metal-organic interfaces*", presented at the International Symposium on Charge Transfer in Metal-Organic Systems at Surfaces, University of Warwick, UK, 11/14/2018.
[14] "*Ab initio simulation of hot-electron mediated chemistry at metal surfaces"*, presented at the 16th international conference on Dynamics, Interactions, and Electronic Transitions at Surfaces (DIET16), Eibsee, Germany, 10/10/2018.
[13] "*Van–der–waals–inclusive tight–binding methods for structure and stability prediction of hybrid organic–inorganic materials*", presented at International Materials Research Conference (IMRC), Cancun Mexico, 08/21/2018.
[12] "*Machine learning beyond energy landscapes for chemical reactions at surfaces*", presented at IPAM Reunion Workshop on "Understanding Many-Particle Systems with Machine Learning", Lake Arrowhead, USA, 06/11/2018.
[11] "*First-principles insights into hot-electron-induced ultrafast dynamics at metal surfaces*", presented at DPG Spring Meeting of the Condensed Matter Section (SKM), Berlin, Germany, 03/13/2018.
[10] "*Electronic friction in chemical dynamics at metal surfaces*", presented at CECAM Workshop "Challenges in reaction dynamics of gas-surface interactions, methodological advances in dissipative, and non-adiabatic processes", Albi, France, 06/27/2017.
[9] "*Collective curvilinear coordinates in interface structure and function prediction*", presented at CECAM Workshop Interface Morphology Prediction with Robust and Efficient Structure Search (IMPRESS), Aalto University, Finland, 06/08/2017.
[8] "*The role of nonadiabatic friction in chemical dynamics at metal surfaces*", presented at DPG Spring Meeting of the Condensed Matter Section (SKM), Dresden, Germany, 03/21/2017.
[7] "*Collective curvilinear coordinates in materials structure search and beyond*", presented at the IPAM Workshop "Machine-Learning meets Many-Particle Problems", Los Angeles, California, 09/28/2016.
[6] "*Tensorial electronic friction and nonadiabatic dynamics in FHI-Aims",* presented at the FHI-aims Developers' and Users' Workshop, Munich, Germany, 07/22/2016.
[5] "*Structure and dynamics of functional molecules on surfaces, presented at the Institute of Physics of the Czech Academy of Sciences*", Prague, Czech Republic, 03/22/2016.
[4] "*Finite-temperature effects on structure and energetics: organic adsorbates from a first principles perspective*", presented at the European Conference on Surface Crystallography and Dynamics (ECSCD-12), Trieste, Italy, 10/19/2015.
[3] "*Ab-initio dynamics of large functional molecules on metal surfaces*", presented at the Gordon Research Conference Dynamics at Surfaces 2015, Newport, RI, USA, 08/13/2015.
[2] "*Many-body interactions in dynamics of molecules on surfaces*", presented at the MMBI 2015 Workshop, Castelleto di Brenzone, Italy, 05/29/2015.
[1] "*First-principles mechanistic insight into molecular switching at metal surfaces: azobenzenes on Ag(111) and Au(111)*", presented at the Central European Symposium on Theoretical Chemistry, CESTC, Znojmo, Czech Republic, 08/27/2013.

List of Invited Departmental Seminar Talks

[34] "*Reaction discovery and chemistry by design with physics-led machine learning*", Max Planck Institute for Multidisciplinary Research, Goettingen, Germany, 04/09/2024
[33] "*Simulation of hot-electron-driven chemistry at surfaces and nanoparticles*", Department of Chemistry, University of Potsdam, Germany, 02/02/2024

[32] "*Machine learning of electronic structure for molecular design*", Seminar at Pfizer AI Research, Berlin, Germany, 02/01/2024
[31] "*Simulation of light- and electron-driven chemistry at surfaces and plasmonic nanoparticles*", Department of Physics, University of Freiburg, Germany, 11/21/2023
[30] "*Machine learning of electronic structure for quantum dynamics and molecular design*", School of Chemistry, University of Bristol, UK, 11/15/2023
[29] "*Machine learning of electronic structure for quantum dynamics and molecular design*", Department of Chemistry, University of York, UK, 04/19/2023
[28] "*Machine-learning-enabled discovery of extreme chemistry*", Department of Chemistry, University of Cambridge, UK, 04/17/2023
[27] "*Machine learning of electronic structure for quantum dynamics and molecular design*", TU Eindhoven, Netherlands, 12/07/2022
[26] "*Deep learning surrogates of electronic structure for quantum dynamics and molecular design*", Seminar of the STFC Scientific Machine Learning (SciML) group, virtual, 10/13/2022
[25] "*Hot electrons in surface chemistry: From molecular scattering to plasmonic catalysis*", Seminar of the Theory Department, Fritz-Haber Institute of the Max Planck Society, Berlin, 06/22/2022
[24] "*Hot electrons in chemical reactions at metal surfaces: From molecular beam scattering to plasmonic chemistry*", Seminar of the Department of Chemistry, University of Cambridge, UK, 02/09/2022
[23] "*Spectroscopic Signatures and Dynamics of Charge Transfer at Metal-Organic Interfaces*", Diamond Light Source Synchrotron Structure and Surfaces Group Seminar, Didcot, UK, 11/01/2021.
[22] "*Computational insights into light- and electron-driven chemistry at surfaces*", presented at the Hutter group seminar at the Department of Chemistry, University of Zurich, Switzerland, 04/26/2021.
[21] *"Machine learning representations of molecular electronic structure: From deep learning of wave functions to big-data-driven quantum chemistry*", presented at the seminar of the Institut für Wissenschaftliches Rechnen, University of Heidelberg, Germany, 04/21/2021.
[20] "Deep learning of molecular wavefunctions and Hamiltonians", presented at the virtual summer seminar series of the Department of Chemistry, Cardiff University, UK, 07/03/2020.
[19] "*Computational insights into light- and electron-driven chemistry at surfaces*", presented at the departmental seminar of the Department of Chemistry, University of Marburg, Germany, 12/10/2019.
[18] "*From photocatalysis to molecular switching: Computational insights into light- and electron-driven chemistry at surfaces*", presented at the departmental seminar of the Department of Chemistry, University of Graz, Austria, 11/15/2019.
[17] "*Computational design of hot-electron catalysts: An 'exciting' path to solar-to-fuel conversion*", presented at the University of Warwick Energy Forum, UK, 05/13/2019.
[16] "*Computational insights into light-and electron-driven chemistry at surfaces*", presented at the Theory of Condense Matter group seminar at the Cavendish Laboratory, Cambridge University, UK, 11/15/2018.
[15] "*Computational insights into light-and electron-driven chemistry at surfaces*", presented at the departmental seminar of the Department of Chemistry, Monash University, Melbourne, Australia, 10/18/2018.
[14] "*Predicting the dynamics and spectroscopic signatures of controlled chemistry at functional metal-organic interfaces*", presented at the seminar of the department of solid state physic, TU Graz, Austria, 09/20/2018.
[13] "*Theory of photon-and electron-stimulated chemistry at surfaces*", presented at departmental seminar, University of Luxembourg, Luxembourg, 01/08/2018.
[12] "*Ab-initio insights into stimulated surface chemistry*", presented at Pittsburgh Quantum Institute, Pittsburgh, Pennsylvania, 02/09/2017.
[11] "*Electronic friction in chemical dynamics at metal surfaces, presented at Connecticut Valley Quantum Chemistry (CVQC) Seminar*", Yale Energy Sciences Institute, New Haven, Connecticut, 01/18/2017.
[10] "*Self-assembly, switching, and catalysis: ab-initio insights into stimulated chemistry on surfaces*", presented at the School of Chemistry and Biochemistry at Georgia Institute of Technology, Atlanta, USA 11/29/2016.
[9] "*Controlled self-assembly, switching, and catalysis: ab-initio insights into stimulated surface chemistry*", presented at the Department of Chemistry and Biochemistry at UCLA, Los Angeles, California, 10/19/2016.
[8] "*Light and electron driven reactions of molecules on surfaces*", presented at the Institut für Physikalische Chemie, University of Göttingen, Germany, 03/01/2016.

[7] "*Structure and dynamics of functional molecules on surfaces*", presented at the Physics and Materials Science Research Unit, Université de Luxembourg, Luxembourg, 02/25/2016.
[6] "*Structure and dynamics of functional molecules on surfaces, presented at the Department of Chemistry*", University of Colorado at Boulder, CO, USA, 02/03/2016.
[5] "*Efficient ab-initio approaches towards the photochemistry of functional molecules on metal surfaces*", presented at the SuperMUC Status and Results Workshop, Leibnitz-Rechenzentrum, Germany, 07/08/2014.
[4] "*First principles mechanistic insight into molecular switching at metal surfaces, presented at the Department of Chemistry*", University of Potsdam, Germany, 01/29/2014.
[3] "*A first-principles description of metal-surface adsorbed isomerization dynamics – azobenzene on coinage metal surfaces*", presented at the group seminar Prof. Lackinger, TU Munich, Germany, 02/08/2013.
[2] "*A first-principles description of metal-surface adsorbed isomerization dynamics – azobenzene on coinage metal surfaces*", presented at the group seminar Prof. Weinelt, Free University Berlin, Germany, 01/18/2013.
[1] "*Thermally induced switching of azobenzene at coinage metal surfaces? bistability loss and balanced functionalization*", presented at the group seminar Prof. Tegeder, Free University Berlin, Germany, 05/04/2012.