Dr. Reinhard J. Maurer

Associate Professor and UKRI Future Leaders Fellow

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Experience

08/2020 – present	**Associate Professor of Computational Chemistry**, University of Warwick, UK	
09/2017 – 07/2020	**Assistant Professor of Computational Chemistry**, University of Warwick, UK	
09/2015 – 11/2015	**Visiting Fellow** at Institute of Pure and Applied Mathematics, UCLA, USA	
11/2014 – 08/2017	**Postdoctoral Associate**, Yale University	group of Prof. John C. Tully
03/2014 – 10/2014	**Postdoctoral Associate**, TU Munich	group of Prof. Karsten Reuter
10/2010 – 02/2014	**Graduate Researcher**, TU Munich	group of Prof. Karsten Reuter
06/2009 – 09/2010	**Undergraduate Researcher**, University of Graz	group of Prof. Alexander Sax
06/2008 – 05/2009	**Undergraduate Researcher**, University of Graz	group of Prof. Otto Glatter

Academic Qualifications

27.01.2014	**PhD in Theoretical Chemistry**, Technical University Munich, Germany graduated *summa cum laude*, Supervisor: Prof. Karsten Reuter
23.06.2010	**Diploma in Chemistry**, University of Graz, Austria passed with highest distinction, GPA: 1.1 (highest: 1.0, lowest: 5.0)

Publication Track Record

A total of **49 publications** in peer-reviewed journals, including:

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

- Two invited first-author reviews on advances in Computational Materials Science
- Two invited articles in special issues on "*Emerging Leaders*" of J. Phys. Condens. Matter (2018,2020)

For details see group publication page: https://preview.tinyurl.com/y2das4zd

Presentation Track Record

Summary: **20 invited talks at international conferences, 22 invited talks at department/university seminars**, 12 contributed conference talks, 12 poster contributions, with highlights including:

2020	ACS Fall Meeting Symposium "From Bench to Market: Leveraging AI & Advanced Computational Methods to Solve Hard Problems", San Francisco, USA
2018	Dynamics, Interactions, and Electronic Transitions at Surfaces (DIET16), Eibsee, Germany
2018	International Materials Research Conference (IMRC), Cancun, Mexico
2017	CECAM Workshop "Interface Morphology Prediction (IMPRESS)", Helsinki, Finland
2017	Spring meeting of the Condensed Matter Section of the German Physical Society (DPG)
2015	Gordon Research Conference on Dynamics at Surfaces, Newport, USA

For details see List of Presentations below

External Grant Income and Fellowships

2020 – (2021)	ARCHER2 eCSE programme funding for 10 Postdoc months, PI	£101,855
2020 – (2021)	Diamond Light Source Collaboration funding for 6 Postdoc months, PI	£22,337
2019 – (2023)	Project funding for PhD studentship from Diamond Light Source, PI	£51,184
2019 – (2023)	**UKRI Future Leaders Fellowship**, PI	£1,432,248
2019 – (2023)	**The Leverhulme Trust**, Research Project Grant, PI	£175,151
2019	6-month PostDoc funding via **EPSRC-funded AI3SD Network+**, PI	£47,908
2018 – (2023)	**6 competitively awarded EPSRC-funded PhD studentships** via (approximate figures including overheads at 100% full economic costing)	

- Centre for Doctoral Training in Diamond Science and Technology (DST CDT) ~£100k
- 2 x Centre for Doctoral Training in Molecular and Analytical Sciences (MAS CDT) ~£200k
- Centre for Doctoral Training in Mathematics for Real-World Systems (MathSys CDT) ~£100k
- DTP PhD studentship funded via National Productivity Investment Fund of UK Government, in collaboration with Merck Ltd. (in-kind contributions) ~£100k
- Centre for Doctoral Training in Modelling of Heterogeneous Systems (Hetsys CDT) with 50% co-funding from Atomic Weapons Establishment (AWE Ltd.) ~£100k

2018 – 2019	Warwick Institute of Advanced Teaching and Learning, Strategic Teaching Project Grant on "A University-wide platform for teaching and learning of computational key skills via interactive notebooks"	£4,152
2018 – 2019	Monash-Warwick Alliance, Research Catalyst Collaboration Fund, PI	£14,934
2018 – 2019	University of Warwick, Research Development Fund, PI	£26,876

Grant Income: ~£2.5M

2011-2020 Numerous HPC time proposals funded via, PRACE, MCC-HEC (EPSRC), UKRI, Bavarian Academy of Science, Helmholtz Research Society, totalling well beyond 50M CPUh.

Prizes

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"

2016 Young Scientist Award of the President of the Technical University Munich
1 price/year across all disciplines/faculties, awarded for
"outstanding research and teaching accomplishments in the area of nanofunctionalized materials and the translation of deep chemical understanding into modern computing algorithms"

2007 – 2010 3 times recipient of the excellence scholarship of the faculty of natural sciences, University of Graz, Austria

2007 – 2010 3 times recipient of the excellence scholarship of the Austrian federal state of Styria

Supervision Track Record

Since 2017 Currently leading a team of **9 PhD students** and **4 PostDocs**, University of Warwick
Past supervision/Alumni: 4 MSc students, 1 PostDoc

2015 – 2016 Cosupervision of 1 PhD student, Yale University

2010 – 2015 Cosupervision of 5 MSc and 5 BSc students, TU Munich and University of Graz

Academic Service and Administration

Since 08/2020 **Editorial Board Member** for

- *Communications Materials* Nature journal
- Frontiers in Catalysis

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 (jointly between Surface Physics, Materials Physics, and Chemical Physics divisions) [COVID cancelled]

04/2019 Organisation of international conference on Computational Molecular Science (CMS2019) at University of Warwick, 165 attendees. Biggest UK conference on computational chemistry.

Since 10/2018 Member of the undergraduate admissions committee for Chemistry at University of Warwick (responsibilities include Marketing coordination and co-organisation of Offer Holder Days)

Since 2018 **External Examiner** at 2 PhD Defences: TU Graz, Austria & University of Leiden, Netherlands

Since 2016 **Grant review activity** for EPSRC, UK Research and Innovation (UKRI), German research funding agency (DFG), Dutch funding agency (NWO), and EC-MSCA programme

02/2015 Organisation of international workshop at Rudolfshuette, Austria on First-Principles-Based Multiscale Modelling in Materials, Energy, and Catalysis

Since 2012 **Peer review activity** for
JACS, Nature Communications, Journal of Chemical Physics, The Journal of Physical Chemistry, The Journal of Physical Chemistry Letters, Physical Review Letters, Physical Review B, Chemical Physics Letters, Computational Materials Science, Journal of Chemical Theory and Computation, Computational Physics Communications, Machine Learning: Science and Technology (IOP), npj Computational Materials, Computational Physics Communications

Research Collaborations

Prof. Hua Guo (University of New Mexico, USA), Prof. Bin Jiang (USTC, China), Prof. Phil Woodruff FRS, Prof. Giovanni Costantini, Prof. Pat Unwin, Prof. Vas Stavros, Prof. Julie Macpherson (U Warwick), Prof. Michael Gottfried (U Marburg, Germany), Dr. David Duncan (Diamond Light Source, UK), Prof. Alexandre Tkatchenko (U Luxembourg), Dr. Christian Wagner and Prof. F. Stefan Tautz (Helmholtz Centre Julich, Germany), Dr. Ben Hourahine (U Strathclyde), Prof. David Yaron (Carnegie Mellon University, USA), Prof. Klaus-Robert Müller (TU Berlin), Prof. Meike Stöhr (U Groningen, NL)

Professional Society Memberships

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)

List of Publications

[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**, "*Deep learning of quantum chemistry to predict the molecular wavefunction and more*", 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**, DOI: 10.1146/annurev–matsci–070218–010143 (2019).

[36] **R. J. Maurer** and K. Reuter, "*Computational design of metal-supported molecular switches: transient ion formation during light- and electron-induced isomerisation of azobenzene*", J. Phys.: Condens. Matter, Invited Article Special Issue "Emerging Leaders" **31**, 044003 (2018).

[35] P. J. Blowey, **R. J. Maurer**, L. A. Rochford, D. A. Duncan, J.-H. Kang, D. A. Warr, A. J. Ramadan, T.-L. Lee, P. K. Thakur, G. Costantini, K. Reuter, and D. P. Woodruff, "*The structure of VOPc on Cu(111): does V=O point up, or down, or both?*", J. Phys. Chem. C **123**, pp. 8101-8111 (2018).

[34] H. Hussein, **R. J. Maurer**, H. Amari, J. Peters, L. Meng, R. Beanland, M. Newton, and J. Macpherson, "*Tracking metal electrodeposition from nucleation and growth of a single atom to a nanoparticle*", ACS Nano **12**, 7388–7396 (2018).

[33] A. Ge, B. Rudshteyn, J. Zhu, **R. J. Maurer**, V. S. Batista, and T. Lian, "*Electron-hole-pair-induced vibrational energy relaxation of rhenium catalysts on gold surfaces*", J. Phys. Chem. Lett. **9**, 406–412 (2018).

[32] M. Mortazavi, J. G. Brandenburg, **R. J. Maurer**, and A. Tkatchenko, "*Structure and stability of molecular crystals with many-body dispersion-inclusive density functional tight binding*", J. Phys. Chem. Lett. **9**, 399–405 (2018).

[31] **R. J. Maurer**, B. Jiang, H. Guo, and J. C. Tully, "*Mode specific electronic friction in dissociative chemisorption on metal surfaces: H_2 on Ag(111)*", Phys. Rev. Lett. **118**, 256001 (2017).

[30] K. Diller, **R. J. Maurer**, M. Müller, and K. Reuter, "*Interpretation of x-ray absorption spectroscopy in the presence of surface hybridization*", J. Chem. Phys. **146**, 214701 (2017).

[29] **R. J. Maurer**, M. Askerka, V. S. Batista, and J. C. Tully, "*Ab-initio tensorial electronic friction for molecules on metal surfaces: nonadiabatic vibrational relaxation*", Phys. Rev. B **94**, 115432 (2016).

[28] K. Krautgasser, C. Panosetti, D. Palagin, K. Reuter, and **R. J. Maurer**, "*Global Structure Search for Molecules on Surfaces: Efficient Sampling with Curvilinear Coordinates*", J. Chem. Phys. **145**, 084117 (2016).

[27] K. Scheil, T. G. Gopakumar, J. Bahrenburg, F. Temps, **R. J. Maurer**, K. Reuter, and R. Berndt, "*Switching of an azobenzene-tripod molecule on Ag(111)*", J. Phys. Chem. Lett. **7**, 2080–2084 (2016).

[26] **R. J. Maurer**, V. G. Ruiz, J. Camarillo-Cisneros, W. Liu, N. Ferri, K. Reuter, and A. Tkatchenko, "*Adsorption structures and energetics of molecules on metal surfaces: Bridging experiment and theory*", Prog. Surf. Sci. Invited Review **91**, 72–100 (2016).

[25] M. Askerka[+], **R. J. Maurer**[+], V. S. Batista, and J. C. Tully, "*Role of tensorial electronic friction in energy transfer at metal surfaces*", Phys. Rev. Lett. Editor's Suggestion **116**, 217601 (2016). [+]Equal contribution

[24] M. Stöhr, G. S. Michelitsch, J. C. Tully, K. Reuter, and **R. J. Maurer**, "*Communication: Charge-Population Based Dispersion Interactions for Molecules and Materials*", J. Chem. Phys. **144**, 151101 (2016).

[23] **R. J. Maurer**, W. Liu, I. Poltavsky, T. Stecher, H. Oberhofer, K. Reuter, and A. Tkatchenko, "*Thermal and electronic fluctuations of flexible adsorbed molecules: Azobenzene on Ag(111)*", Phys. Rev. Lett. **116**, 146101 (2016).

[22] J. A. Lloyd, A. C. Papageorgiou, S. Fischer, S. C. Oh, O. Saglam, K. Diller, D. A. Duncan, F. Allegretti, F. Klappenberger, M. Stöhr, **R. J. Maurer**, K. Reuter, J. Reichert, and J. V. Barth, "*Dynamics of Spatially Confined Bisphenol A Trimers in a Unimolecular Network on Ag(111)*", Nano Lett. **16**, 1884–1889 (2016).

[21] S. Karan, N. Li, Y. Zhang, Y. He, I.-P. Hong, H. Song, J.-T. Lü, Y. Wang, L. Peng, K. Wu, G. S. Michelitsch, **R. J. Maurer**, K. Diller, K. Reuter, A. Weismann, and R. Berndt, "*Spin Manipulation by Creation of Single-Molecule Radical Cations*", Phys. Rev. Lett. **116**, 027201 (2016).

[20] M. Müller, K. Diller, **R. J. Maurer**, and K. Reuter, "*Interfacial charge rearrangement and intermolecular interactions: Density-functional theory study of free-base porphine adsorbed on Ag(111) and Cu(111)*", J. Chem. Phys. **144**, 024701 (2016).

[19] C. Panosetti, K. Krautgasser, D. Palagin, K. Reuter, and **R. J. Maurer**, "*Global materials structure search with chemically-motivated coordinates*", Nano Lett. **15**, 8044–8048 (2015).

[18] **R. J. Maurer**, V. G. Ruiz, and A. Tkatchenko, "*Many-body dispersion effects in the binding of adsorbates on metal surfaces*", J. Chem. Phys. **143**, 102808 (2015).

[17] F. Blobner, P. N. Abufager, R. Han, J. Bauer, D. A. Duncan, **R. J. Maurer**, K. Reuter, P. Feulner, and F. Allegretti, "*Thiolate-Bonded Self-Assembled Monolayers on Ni(111): Bonding Strength, Structure, and Stability*", J. Phys. Chem. C **119**, 15455–15468 (2015).

[16] M. Willenbockel, **R. J. Maurer**, C. Bronner, M. Schulze, B. Stadtmüller, S. Soubatch, P. Tegeder, K. Reuter, and F. S. Tautz, "*Coverage-driven dissociation of azobenzene on Cu(111): a route towards defined surface functionalization*", Chem. Commun. **15**, 15324–15327 (2015).

[15] Z. Wang, L. Heinke, J. Jelic, M. Cakici, M. Dommaschk, **R. J. Maurer**, H. Oberhofer, S. Grosjean, R. Herges, S. Bräse, and Others, "*Photoswitching in nanoporous, crystalline solids: an experimental and theoretical study for azobenzene linkers incorporated in MOFs*", Phys. Chem. Chem. Phys. **17**, 14582– 14587 (2015).

[14] K. Diller, F. Klappenberger, F. Allegretti, A. C. Papageorgiou, S. Fischer, D. A. Duncan, **R. J. Maurer**, J. A. Lloyd, S. C. Oh, K. Reuter, and J. V. Barth, "*Temperature-dependent templated growth of porphine thin films on the (111) facets of copper and silver*", J. Chem. Phys. **141**, 144703 (2014).

[13] J. Hoja, **R. J. Maurer**, and A. F. Sax, "*Adsorption of Glucose, Cellobiose, and Cellotetraose onto Cellulose Model Surfaces*", J. Phys. Chem. B **118**, 9017–9027 (2014).

[12] G. Mercurio, **R. J. Maurer**, S. Hagen, F. Leyssner, J. Meyer, P. Tegeder, S. Soubatch, K. Reuter, and F. S. Tautz, "*X-ray standing wave simulations based on fourier vector analysis as a method to retrieve complex molecular adsorption geometries*", Front. Phys. **2**, 2 (2014).

[11] G. Mercurio, **R. J. Maurer**, W. Liu, S. Hagen, F. Leyssner, P. Tegeder, J. Meyer, A. Tkatchenko, S. Soubatch, K. Reuter, and F. S. Tautz, "*Quantification of finite-temperature effects on adsorption geometries of-conjugated molecules: Azobenzene/Ag(111)*", Phys. Rev. B **88**, 035421 (2013).

[10] **R. J. Maurer** and K. Reuter, "*Excited-state potential-energy surfaces of metal-adsorbed organic molecules from linear expansion Δ-self-consistent field density-functional theory (ΔSCF-DFT)*", J. Chem. Phys. **139**, 014708 (2013).

[9] T. G. Gopakumar, T. Davran-Candan, J. Bahrenburg, **R. J. Maurer**, F. Temps, K. Reuter, and R. Berndt, "*Broken Symmetry of an Adsorbed Molecular Switch Determined by Scanning Tunneling Spectroscopy*", Angew. Chem. Int. Ed. **52**, 11007–11010 (2013).

[8] **R. J. Maurer**, A. F. Sax, and V. Ribitsch, "*Molecular simulation of surface reorganization and wetting in crystalline cellulose I and II*", Cellulose **20**, 25–42 (2013).

[7] R. J. Maurer and K. Reuter, "*Bistability Loss as a Key Feature in Azobenzene (Non-) Switching on Metal Surfaces*", Angew. Chem. Int. Ed. **51**, 12009–12011 (2012).

[6] S. Engelskirchen, **R. J. Maurer**, T. Levy, R. Berghaus, H. Auweter, and O. Glatter, "*Emulsified Microemulsions as Solvent-free Carrier for an Amorphous Solid Plant Protection Agent*", Chem. Lett. **41**, 1125–1127 (2012).

[5] S. Engelskirchen, **R. J. Maurer**, T. Levy, R. Berghaus, H. Auweter, and O. Glatter, "*Highly concentrated emulsified microemulsions as solvent-free plant protection formulations.*", J. Colloid Interface Sci. **388**, 151–61 (2012).

[4] S. Engelskirchen, **R. J. Maurer**, and O. Glatter, "*Effect of glycerol addition on the internal structure and thermal stability of hexosomes prepared from phytantriol*", Colloids Surf., A **391**, 95–100 (2011).

[3] **R. J. Maurer** and K. Reuter, "*Assessing computationally efficient isomerization dynamics: ΔSCF densityfunctional theory study of azobenzene molecular switching.*", J. Chem. Phys. **135**, 224303 (2011).

[2] **R. J. Maurer** and A. Sax, "*Solvation of carbon nanotubes by aniline calculated with density functional tight binding*", Phys. Chem. Chem. Phys.: PCCP **12**, 9893–9899 (2010).

[1] **R. J. Maurer** and A. Sax, "*Molecular dynamics of cellulose crystal surfaces with ChemShell*", Proc. Comp. Sci. **1**, 1149–1154 (2010).

List of Presentations

Only first-author contributions are listed

List of Invited Talks

[42] **R. J. Maurer**, *"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.

[41] **R. J. Maurer**, "A deep neural network to represent molecular wave functions" presented at the virtual MACSIM 2020 workshop, 06/29 – 07/02/2020.

[39] **R. J. Maurer**, "*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.

[38] **R. J. Maurer**, "*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.

[37] **R. J. Maurer**, *"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.

[36] **R. J. Maurer**, "*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.

[35] **R. J. Maurer**, "*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.

[34] **R. J. Maurer**, **"***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

[33] K. T. Schütt, M. Gastegger, A. Tkatchenko, K.-R. Müller, **R. J. Maurer,** "*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.

[32] **R.J. Maurer**, "*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.

[31] **R. J. Maurer,** "*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.

[30] **R. J. Maurer,** "*A first-principles perspective on the electronic and spectroscopic signatures of charge transfer at metal-organic interfaces*", presented at the Symposium on Charge Transfer in Metal-Organic Systems at Surfaces, University of Warwick, UK, 11/14/2018.

[29] **R. J. Maurer,** "*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.

[28] **R. J. Maurer, "***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.

[27] **R. J. Maurer, "***Predicting the dynamics and spectroscopic signatures of controlled chemistry at functional metal-organic interfaces*", presented at the departmental seminar of the department of solid state physic at the TU Graz, Austria, 09/20/2018.

[26] **R. J. Maurer, "***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.

[25] **R. J. Maurer, "***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.

[24] **R. J. Maurer,** "*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.

[23] **R. J. Maurer,** "*Theory of photon-and electron-stimulated chemistry at surfaces*", presented at departmental seminar, University of Luxembourg, Luxembourg, 01/08/2018.

[22] **R. J. Maurer, "***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.

[21] **R. J. Maurer,** "*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.

[20] **R. J. Maurer, "***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.

[19] **R. J. Maurer, "***Ab-initio insights into stimulated surface chemistry*", presented at Pittsburgh Quantum Institute, Pittsburgh, Pennsylvania, 02/09/2017.

[18] **R. J. Maurer, "***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.

[17] **R. J. Maurer, "***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, Georgia, USA 11/29/2016.

[16] **R. J. Maurer, "***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.

[15] **R. J. Maurer, "***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.

[14] **R. J. Maurer, "***Tensorial electronic friction and nonadiabatic dynamics in FHI-Aims",* presented at the FHI-aims Developers' and Users' Workshop, Munich, Germany, 07/22/2016.

[13] **R. J. Maurer, "***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.

[12] **R. J. Maurer, "***Light and electron driven reactions of molecules on surfaces*", presented at the Institut für Physikalische Chemie, University of Göttingen, Germany, 03/01/2016.

[11] **R. J. Maurer, "***Structure and dynamics of functional molecules on surfaces*", presented at the Physics and Materials Science Research Unit, Université de Luxembourg, Luxembourg, 02/25/2016.

[10] **R. J. Maurer, "***Structure and dynamics of functional molecules on surfaces, presented at the Department of Chemistry*", University of Colorado at Boulder, CO, USA, 02/03/2016.

[9] **R. J. Maurer, "***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.

[8] **R. J. Maurer, "***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.

[7] **R. J. Maurer, "***Many-body interactions in dynamics of molecules on surfaces*", presented at the MMBI 2015 Workshop, Castelleto di Brenzone, Italy, 05/29/2015.

[6] **R. J. Maurer, "***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.

[5] **R. J. Maurer** and K. Reuter, "*First principles mechanistic insight into molecular switching at metal surfaces, presented at the Department of Chemistry*", University of Potsdam, Germany, 01/29/2014.

[4] **R. J. Maurer** and K. Reuter, "*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.

[3] **R. J. Maurer, "***A first-principles description of metal-surface adsorbed isomerization dynamics – azobenzene on coinage metal surfaces*", presented at the group seminar Prof. Lackinger, Technical University Munich, Germany, 02/08/2013.

[2] **R. J. Maurer, "***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] **R. J. Maurer, "***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.

List of Contributed Talks

[12] **R. J. Maurer,** "*Electrochemically-driven metal nanoparticle nucleation and growth*", presented at the International Workshop on Computational Electrochemistry (IWCE), Aalto University, Finland, 07/12/2018.

[11] **R. J. Maurer, "***Computational design of functional hybrid organic-inorganic interfaces: from single molecule control to surface self-assembly*", presented at the "Recent Appointees in Material Science Conference" (RAMS2017), University of Exeter, UK, 09/12/2017.

[10] **R. J. Maurer,** W. Liu, I. Poltavskyi, T. Stecher, H. Oberhofer, A. Tkatchenko, and K. Reuter, "*Mind the entropy: electronic and thermal fluctuations of large molecules on metals*", presented at the APS March meeting, San Antonio, USA, 03/03/2015.

[9] **R. J. Maurer, "***Term-by-term construction of ab initio many-body potentials for dynamics on surfaces: hydrogen on Pd(100)*", presented at the Winter Workshop Rudolfshütte 2015, Uttendorf, Austria, 01/28/2015.

[8] **R. J. Maurer,** M. Stöhr, and K. Reuter, "*Molecular switching of azobenzene: towards design strategies for functioning molecular switches*", presented at the DPG Spring Meeting of the Condensed Matter Section (SKM), Dresden, Germany, 04/03/2014.

[7] **R. J. Maurer** and K. Reuter, "*Towards a mechanistic understanding of photoinduced (non-)switching of metal surface adsorbed azobenzenes*", presented at the International Symposium on Theoretical Chemical Physics, ISTCP, Budapest, Hungary, 09/23/2013.

[6] **R. J. Maurer** and K. Reuter, "*Computationally efficient excited states of hybrid organic/inorganic systems: dynamics and spectroscopy with delta-self-consistent-field density-functional theory (deltascf-dft)*", presented at the DPG Spring Meeting of the Condensed Matter Section (SKM), Regensburg, Germany, 03/12/2013.

[5] **R. J. Maurer** and K. Reuter, "*Lost bistability: how surface adsorption can prevent molecular switching at metal surfaces*", presented at the 29th European Conference on Surface Science (ECOSS), Edinburgh, United Kingdom, 09/06/2012.

[4] **R. J. Maurer** and K. Reuter, "*Thermally induced switching of azobenzene at coinage metal surfaces? bistability loss and balanced functionalization*", presented at the DPG Spring Meeting of the Condensed Matter Section (SKM), Berlin, Germany, 03/28/2012.

[3] **R. J. Maurer,** E. Deront, and K. Reuter, "*Towards isomerization dynamics of adsorbed molecular switches: a ΔSCF density-functional theory study*", presented at the DPG Spring Meeting of the Condensed Matter Section (SKM), Dresden, Germany, 03/15/2011.

[2] **R. J. Maurer** and A. Sax, "*Molecular dynamics of cellulose crystal surfaces with chemshell, presented at the 10th International Conference on Computational Science (ICCS)*", Amsterdam, The Netherlands, 06/01/2010.

[1] **R. J. Maurer** and A. Sax, "*Solvation of single walled carbon nanotubes in aromatics as predicted by density-functional tight binding*", presented at the Workshop on Theoretical Chemistry, Mariapfarr, Austria, 02/19/2010.

List of Poster Presentations

[12] **R. J. Maurer,** B. Jiang, H. Guo, and J. C. Tully, "*Electronic friction effects in dissociative chemisorption on metal surfaces"*, presented at the Gordon Research Conference (GRC) Dynamics at Surfaces 2017, Newport, RI, USA, 07/30/2017.

[11] **R. J. Maurer,** M. Askerka, and J. C. Tully, "*Nonadiabatic coupling in dynamics of molecules at surfaces"*, presented at the Gordon Research Seminar (GRS) Dynamics at Surfaces 2015, Newport, RI, USA, 08/08 – 08/09/2015.

[10] **R. J. Maurer,** M. Stöhr, and K Reuter*, "Ab-initio molecular device design: from electronic structure to optimal decoupling strategies*", presented at the 563rd WE-Heraeus-Seminar: Functional Molecules at Surfaces, Bad Honnef, Germany, 05/19 – 05/21/2014.

[9] **R. J. Maurer** and K. Reuter, "*An efficient static dft approach to excited states of large organic adsorbates: azobenzenes on coinage metals"*, presented at the 15th International Conference on Density Functional Theory and its Applications, DFT, Durham, United Kingdom, 09/09 – 09/13/2013.

[8] **R. J. Maurer** and K. Reuter*, "A first-principles description of metal-surface mounted molecular switching: azobenzenes on coinage metals"*, presented at the Workshop "Controlled Atomic Dynamics on Solid Surfaces: Atom and Molecular Manipulation", San Sebastian, Spain, 05/13 – 05/16/2013.

[7] **R. J. Maurer** and K Reuter, *"DeltaSCF-DFT: an efficient alternative for dynamics and spectroscopy of adsorbed molecular switches?!"*, presented at the XV International Workshop on Computational Physics, Materials Science: Total Energy, and Force Methods, Trieste, Italy, 01/13 – 01/15/2013.

[6] **R. J. Maurer** and K Reuter, "*Linear expansion DeltaSCF-DFTt: an efficient alternative for isomerization dynamics of adsorbed molecular switches*", presented at the 5th International Workshop, Summer School on Time-Dependent Density-Functional Theory: Prospects, and Applications, Benasque, Spain, 01/03 - 01/17/2012.

[5] **R. J. Maurer** and K Reuter, "*Towards the isomerization dynamics of adsorbed molecular switches: a ΔSCF density-functional theory study*", presented at the International Workshop on Elementary Processes in Solids and at Interfaces, Kloster Banz, Germany, 05/29 – 06/01/2011.

[4] **R. J. Maurer** and A. Sax, "*Surface reorganisation and wetting of crystalline cellulose I and II*", presented at the Symposium on Theoretical Chemistry (STC), Münster, Germany, 09/26 – 09/30/2010.

[3] **R. J. Maurer** and A. Sax, "*Matching force field energetics and dynamics to density functional tight binding results for carbon nanotube solvation*", presented at the CCP5 Methods in Molecular Simulation Summer School, Belfast, United Kingdom, 07/08 – 07/27/2010.

[2] **R. J. Maurer** and A. Sax, "*Solvation process of single walled carbon nanotubes in aniline*", presented at the International Symposium on Theoretical and Computational Chemistry, Mühlheim an der Ruhr, Germany, 02/28 – 03/02/2010.

[1] **R. J. Maurer** and A. Sax, "*Solvation process of single walled carbon nanotubes in aniline*", Presented at the Central European Symposium on Theoretical Chemistry (CESTC), Dobogókö, Hungary, 09/25 – 09/28/2009.