Curriculum vitae of
Lukas Hörmann

Personal information

Personal address	54 Charminster Drive, Coventry, CV3 5AB, UK
Research institution	Departments of Chemistry and Physics, University of Warwick
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Publication list	google scholar
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Experience

September 2023 – Ongoing	**Marie Curie Researcher Fellow** University of Warwick, Coventry, UK
	• Research into atom-scale energy dissipation mechanisms as a function of the geometric, chemical, and physical properties of surfaces • Co-supervisor of master and PhD theses
May 2022 – August 2023	**Postdoctoral Researcher** Graz University of Technology, Graz, Austria
	• Research of dynamic sliding friction at the nanoscale • Co-supervisor of master theses
April 2018 – April 2022	**Research Assistant** Graz University of Technology, Graz, Austria
	• Development of machine-learning algorithms for surface structure determination and prediction of structure-to-property relationships • Investigation of structures and properties of organic/inorganic interfaces • Co-supervisor of bachelor and master theses
October 2014 – March 2018	**Teaching Assistant** Graz University of Technology, Graz, Austria
	• Supervisor of laboratory exercises and mathematics exercises
April 2009 – July 2011	**Assistant Civil Engineer** Ingenieurbüro Moser GmbH & Co KG, St. Johann, Austria
	• Planning and management of the construction of water-supply facilities and sewage systems • Inspection of water-supply facilities and testing of drinking-water quality

Education

August 2018 – May 2022	**PhD in Technical Sciences** Graz University of Technology, Graz, Austria
	• Structure search for organic/inorganic interfaces using coarse grained modelling and machine learning • Supervisor: Prof. Oliver T. Hofmann
December 2015 – July 2018	**MSc in Technical Sciences** Graz University of Technology, Graz, Austria
	• Overcoming the configurational explosion for surface structure search by coarse grained modeling and Bayesian learning • Supervisor: Prof. Oliver T. Hofmann

October 2011 – November 2015	**BSc in Technical Sciences** Graz University of Technology, Graz, Austria
	• Electronic structure of $CaCuO_2$ in the LSDA+U approximation • Supervisor: Prof. Lilia Boeri
September 2003 – June 2008	**High School Certificate (Matura)** HTL Saalfelden, Saalfelden, Austria

Journal articles

Articles in well-recognised international journals; These publications have received more than 200 citations and an h-index of 7.

1. **Hörmann, L.**, Cartus, J. J., Hofmann, O. T. (2023). *Impact of Static Distortion Waves on Superlubricity.* ACS Omega. doi.org/10.1021/acsomega.3c05044
2. Cartus, J. J., Jeindl, A., Werkovits, A., **Hörmann, L.**, Hofmann, O. T. (2023). *Polymorphism mediated by electric fields: a first principles study on organic/inorganic interfaces.* Nanoscale Advances, 5(8), 2288-2298. doi.org/10.1039/D2NA00851C
3. Berger, R. K., Jeindl, A., **Hörmann, L.**, Hofmann, O. T. (2022). *Role of Adatoms for the Adsorption of F4TCNQ on Au (111).* The Journal of Physical Chemistry C, 126(17), 7718-7727. doi.org/10.1021/acs.jpcc.2c00994
4. Calcinelli, F., Jeindl, A., **Hörmann, L.**, Ghan, S., Oberhofer, H., Hofmann, O. T. (2022). *Interfacial charge transfer influences thin-film polymorphism.* The Journal of Physical Chemistry C, 126(5), 2868-2876. doi:10.1021/acs.jpcc.1c09986
5. **Hörmann, L.**, Jeindl, A., Hofmann, O. (2022). *From a bistable adsorbate to a switchable interface: tetrachloropyrazine on Pt (111).* Nanoscale, 14, 5154-5162. doi: 10.1039/D1NR07763E
6. Jeindl, A., **Hörmann, L.**, Hofmann, O. T. (2022). *How much does surface polymorphism influence the work function of organic/metal interfaces?* Applied Surface Science, 575, 151687. doi: 10.1016/j.apsusc.2021.151687
7. Werkovits, A., Jeindl, A., **Hörmann, L.**, Cartus, J. J., Hofmann, O. T. (2021). *Toward Targeted Kinetic trapping of organic–inorganic interfaces: A computational case study.* ACS Physical Chemistry Au. doi: 10.1021/acsphyschemau.1c00015
8. Jeindl, A., Domke, J., **Hörmann, L.**, Sojka, F., Forker, R., Fritz, T., Hofmann, O. T. (2021). *Nonintuitive surface self-assembly of functionalized molecules on Ag (111).* ACS Nano, 15(4), 6723-6734. doi: 10.1021/acsnano.0c10065
9. Hofmann, O. T., Zojer, E., **Hörmann, L.**, Jeindl, A., Maurer, R. J. (2021). *First-principles calculations of hybrid inorganic–organic interfaces: from state-of-the-art to best practice.* Physical Chemistry Chemical Physics, 23(14), 8132-8180. 10.1039/D0CP06605B
10. **Hörmann, L.**, Jeindl, A., Hofmann, O. T. (2020). *Reproducibility of potential energy surfaces of organic/metal interfaces on the example of PTCDA on Ag (111).* The Journal of Chemical Physics, 153(10), 104701. doi: 10.1063/5.0020736
11. Egger, A. T., **Hörmann, L.**, Jeindl, A., Scherbela, M., Obersteiner, V., Todorovic, M., ..., Hofmann, O. T. (2020). *Charge transfer into organic thin films: A deeper insight through machine-learning-assisted structure search.* Advanced Science, 7(15), 2000992. doi: 10.1002/advs.202000992
12. **Hörmann, L.**, Jeindl, A., Egger, A. T., Scherbela, M., Hofmann, O. T. (2019). *SAMPLE: Surface structure search enabled by coarse graining and statistical learning.* Computer Physics Communications, 244, 143-155. doi: 10.1016/j.cpc.2019.06.010
13. Wruss, E., Hörmann, L., Hofmann, O. T. (2019). Impact of surface defects on the charge transfer at inorganic/organic interfaces. The Journal of Physical Chemistry C, 123(12), 7118-7124.
14. Scherbela, M., **Hörmann, L.**, Jeindl, A., Obersteiner, V., Hofmann, O. T. (2018). *Charting the energy landscape of metal/organic interfaces via machine learning.* Physical Review Materials, 2(4), 043803. doi: 10.1103/PhysRevMaterials.2.043803
15. Obersteiner, V., Scherbela, M., Hörmann, L., Wegner, D., Hofmann, O. T. (2017). Structure prediction for surface-induced phases of organic monolayers: overcoming the combinatorial bottleneck. Nano letters, 17(7), 4453-4460.

Funding

Marie Skłodowska-Curie Postdoctoral Fellowship	
Funding body	UKRI Horizon Guarantee
Project title	Atomic-scale design of superlubricity of carbon nanostructures on metallic substrates
Project duration	September 2023 – August 2025
Amount	**220 908.48 €**
Erwin Schrödinger Fellowship	
Funding body	FWF - Austrian Science Fund
Project title	Nanoscale design of superlubricating interfaces
Project duration	-
Amount	**198 630.000 €**

**Declined in favour of Marie Skłodowska-Curie Postdoctoral Fellowship*

UFO fellowship	
Funding body	Land Steiermark, Abteilung 12 Wirtschaft, Tourismus, Wissenschaft und Forschung
Project title	Schaltbare Superschmierfähigkeit (Switchable superlubricity)
Project duration	September 2022 – August 2023
Amount	**95 313.00 €**
Competitive Initial Funding Programme	
Funding body	Graz University of Technology
Project title	Switchable superlubricity using organic/inorganic interfaces
Project duration	June 2022 – May 2023
Amount	**5 410.00 €**

Conference presentations

Invited talks

- Warwick centre of predictive modelling seminar, University of Warwick, UK (2023)
- Seminar of the Institute of Experimental Physics, University of Regensburg, Germany (2022)
- Seminar Series of the Computational Surface Chemistry Group, University of Warwick, UK (2022)

Contributed talks

- German Physical Society Spring Meeting, Dresden, Germany (2023)
- American Chemical Society Spring Meeting, Virtual (2022)
- American Physical Society March Meeting, Virtual (2022)
- International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering, Virtual (2021)
- American Physical Society March Meeting, Virtual (2021)
- Machine Learning for Materials Science Workshop, Helsinki, Finland (2019)
- German Physical Society Spring Meeting, Regensburg, Germany (2019)
- Austrian Physical Society Meeting, Graz, Austria (2018)
- German Physical Society Spring Meeting, Regensburg, Germany (2018)

Supervision and mentorship

(Co-)supervisor for two master and two bachelor theses with the following titles in the group of Prof. Oliver T. Hofmann at Graz University of Technology:

- **Transfer learning on organic/inorganic interfaces for different substrates** (Master thesis, 2022)
- **Predicting the 5-dimensional potential energy surface of organic molecule adsorption on inorganic substrates** (Master thesis, 2020/2021)

- **Minimum energy paths and barriers on potential energy surfaces predicted with Gaussian process regression** (Bachelor thesis, 2020)
- **Kernel determination for Gaussian process regression of the adsorption potential for molecule bending and adsorption height** (Bachelor thesis, 2018)

Mentor to a PhD student who works in the group of Prof. Egbert Zojer at Graz University of Technology.

Teaching activities

- Exercise course in mathematics 2 for structural engineering students
- Laboratory exercise course (experimental physics 1 and 2) for physics students

Conference organisation

Computational material physics workshop 2023

Location	Schladming, Austria
Dates	May 15 – 17, 2023
Description	Multi-disciplinary workshop that brought together researchers from mathematics as well as experimental, theoretical, and solid-state physics to present their work and discussed new collaborations

Computational material physics workshop 2022

Location	Mönichwald, Austria
Dates	June 20 – 22, 2022
Description	Multi-disciplinary workshop that brought together researchers from experimental, theoretical, and solid-state physics to present their work and discussed new collaborations

Software projects

SAMPLE Structure Search Code

I have developed the SAMPLE structure search code, which is the world's first software package that enables quasi-deterministic surface structure search by using coarse-grained modelling and machine learning. The development started in 2017 and the code is still being constantly improved and updated. The code is written in Python and is available as an open-source pip-package.

FHI-aims Density Functional Theory Code

Additionally, I have contributed to the FHI-aims quantum chemistry code 3 in 2019. The FHI-aims code is written in Fortran.

Transferable skills

- **Research Integrity**, University of Warwick (2023)
- **Financial Regulations & Procedures**, University of Warwick (2023)
- **Anti-Bribery Essentials**, University of Warwick (2023)
- **Equality, Diversity and Inclusion**, University of Warwick (2023)
- **Rhetoric for Talks and Meetings**, Graz University of Technology (2020)
- **Scientific Writing in English**, Graz University of Technology (2020)
- **Inventions, Patents, and Technology Exploitation**, Graz University of Technology (2020)