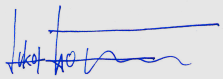
Curriculum vitae of
Lukas Hörmann

Personal information

Personal address	54 Charminster Drive, Coventry, CV3 5AB, UK
Research institution	Departments of Chemistry and Physics, University of Warwick
ORCID-ID	0000-0003-4150-1592
Publication list	google scholar
Website	https://warwick.ac.uk/.../lukas/
Last updated	March 25, 2024
Signature	

Experience

September 2023 – Ongoing	**Marie Curie Research 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 modelling 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

Funding

EuroHPC JU grant	
Funding body	Partnership for Advanced Computing in Europe (PRACE)
Project title	Topologically Designed Defective Graphene for Single Atom Catalysis and Atomic-Scale Friction Engineering
Project duration	March 2024 – April 2025
Amount	**40 million CPU-hours**
**Co-Principal Investigator*	
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	**198 630.00 €**
**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 organisation and administration activities

Organiser of team building and group events	
Dates	2024 – ongoing
Description	Fostering a welcome, respectful, and inclusive environment of students and group members by organising engaging recreational events
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

Public engagement and evidence of esteem

Prices

- Finalist for the Gerhard Ertl Young Investigator Award, German Physical Society condensed matter division spring meeting, DE, 2024
- Best poster award at the Chemistry Postdoctoral Symposium, University of Warwick, UK, 2024

Invited talks

- German Physical Society condensed matter division spring meeting, Berlin, DE, 2024
- Seminar of the Institute of Solid State Physics, Graz University of Technology, AT, 2024
- Warwick Centre of Predictive Modelling seminar, University of Warwick, UK, 2023
- Seminar of the Institute of Experimental Physics, University of Regensburg, DE, 2022
- Seminar Series of the Computational Surface Chemistry Group, University of Warwick, UK, 2022

Invited panel discussions

- Accolade event on European funding and MSCA Postdoc Fellowships, University of Warwick, UK, 2024

Contributed talks

- German Physical Society condensed matter division spring meeting, Dresden, DE, 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, FI, 2019
- German Physical Society condensed matter division spring meeting, Regensburg, DE, 2019
- Austrian Physical Society Meeting, Graz, Austria, 2018
- German Physical Society condensed matter division spring meeting, Berlin, DE, 2018

Teaching, supervision and mentorship

Teaching of exercise classes, tutorials, and lab courses.

- Tutorials in “Electrons in molecules and solids theory of chemical bonding” (2024)
- Exercise course in “Mathematics 2 for structural engineering students” (2017)
- Laboratory exercise course (Experimental physics 1 and 2) for physics students (2014-2018)

(Co-)supervisor of on PhD student in the group of Prof. Reinhard J. Maurer at the University of Warwick.

- **Preliminary title: Phase diagram determination for iron-niobium alloys and defective graphene** (PhD thesis, 2024 – ongoing)

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

- 2022 – ongoing

(Co-)supervisor of 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)

Memberships

Associate fellow of the Institute of Advanced Study at the University of Warwick

Dates	2024 – ongoing
Description	Promote a positive research culture by acknowledging and valuing colleagues for their contributions, fostering mutual support for success, and ensuring the creation of outputs that uphold the highest standards of academic rigor

Member of the DAEMON cost action

Dates	2024 – ongoing
Description	Building a scientific community for the advancement of data-driven applications towards the engineering of functional materials

Member of the German Physical Society

Dates	2017 – ongoing
Description	Public engagement via conference presentations

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 contributed to the FHI-aims quantum chemistry code 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)

References

- **Prof Reinhard J. Maurer**, R.Maurer@warwick.ac.uk
- **Assoc Prof Oliver T. Hofmann**, o.hofmann@tugraz.at
- **Dr Alfred John Weymouth**, jay.weymouth@ur.de
- **Prof Egbert Zojer**, egbert.zojer@tugraz.at