# Curriculum Vitae


## Johannes Laurin Hörmann

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born on 29th June 1988
German

## Research

My research focuses on the multiscale modeling of interfacial phenomena in tribological and electrochemical systems. I combine continuum approaches (finite element solutions of coupled Poisson–Nernst–Planck equations), atomistic simulations (molecular dynamics, DFTB, and DFT), and data-driven methods to understand friction, adsorption, lubrication, and electrochemical double layers at rough and chemically complex interfaces.

A central theme of my work is the frictional behavior of surfactant adsorption films and electrolyte-lubricated contacts under mechanical and electrical stimuli. I develop reproducible, high-performance computational workflows for large-scale simulations and integrate research data management as a core scientific principle. Beyond physics-based modeling, I apply Gaussian process regression and classification to predict surface performance from topographical descriptors, bridging fundamental simulation with industrial surface engineering applications.

My long-term research vision is to establish reproducible, multiscale digital twins of functional interfaces by tightly coupling physics-based simulation, machine learning, and FAIR research data infrastructures.

## Selected Projects

- **Fugaku Junior Researchers (Small-Scale) Project: The influence of molecular design on tribological performance on the nanoscale**
  Principal investigator of Fugaku HPC project that will establish a molecular-level framework linking structure, adsorption, and friction for polyalkylmethacrylate polymer additives and phosphatidylcholine lipid films. Awarded 432,000 node hours.
- **Joint Research Advancement Program University of Freiburg & Nagoya University (2026–2027)**
  Co-author of the funded bilateral research proposal establishing an international collaboration on multiscale modeling of functional interfaces. The project strengthens long-term cooperation between Germany and Japan and advances reproducible computational approaches to complex interfacial systems.
- **Co-founder & CTO, Surface Design Solutions and KTUR Summer School Entrepreneurship: Best Project Award (2022–2023)**
  Led the technical development of machine learning models (Gaussian Process Regression and Classification) for predicting tribological surface performance from topographical data. Translated physics-based simulation insights into industrially deployable predictive tools for surface engineering applications.
- **DFG-funded “AWEARNESS” Project (2024–2025)**
  Contributed to proposal coordination and scientific development of a research initiative investigating tribo-induced formation mechanisms of zinc phosphate glasses derived from ZDDP additives. The project integrates density functional theory (DFT), molecular dynamics (MD), and continuum scale simulations with tribological experiments to understand film growth and wear.

## Skills & Qualifications

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| languages | **German** native, **English** fluent, **Chinese** fluent |
| simulation methods | Finite Elements Method (**FEM**) with **COMSOL**, **ANSYS**, and **FEniCSx** |
| | Molecular Dynamics (**MD**) by **GROMACS** and **LAMMPS** |
| | Density Functional-based Tight Binding (**DFTB**) with **Atomistica** |
| | Density Functional Theory (**DFT**) with **CASTEP** |
| machine learning | Gaussian process regression & classification (**GPR**, **GPC**) with **gpflow** and **sklearn** |
| big data | Computational Workflow Management with **FireWorks** and **snakemake** |
| | Research Data Management with **dtool** & **dserver** |
| visualization | Publication quality figures of continuous and discrete datasets with **matplotlib**, **seaborn**, **OVITO**, **VMD** and **PyMOL** |
| DevOps skills | Github CI/CD, OpenStack, Docker, Podman, Singularity, Make, CMake, EasyBuild, lmod, Slurm, MongoDB, SQL databases, Flask, REST API |
| other tech skills | Python, C/C++, tcl, Lua, MATLAB, Mathematica, LaTeX |

## Education

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|---|---|
| 07/2017 to 07/2025 | **Ph.D. Microsystems Engineering**<br>Simulation, Dept. of Microsystems Engineering (IMTEK), University of Freiburg, Germany |
| | Dissertation (magna cum laude, https://doi.org/10.6094/UNIFR/269291):<br>*Friction of Adsorption Films with Reproducible Molecular Dynamics* |
| 09/2014 to 01/2017 | **Master Mechanical Engineering** (Double Degree Master Program)<br>Dept. of Mechanical Engineering, Tsinghua University, Beijing, China |
| | Master thesis (grade 1.3, German scale):<br>*Computational Multiscale Modeling of the Bipolar Electrochemical Process* |
| 09/2012 to 03/2017 | **Master Engineering Science** (grade 1.6, German scale)<br>Faculty V – Mechanical Engineering and Transport Systems, Technische Universität Berlin, Germany |
| | Foci: Mechatronics, Numerics & Simulation |
| 09/2008 to 09/2012 | **Bachelor Physics** (grade 2.0, German scale)<br>Dept. of Physics, Freie Universität Berlin, Germany |
| | Bachelor thesis (grade 1.0, German scale):<br>*Large Scale Parallel Simulation of EPR Lineshape Spectra* |
| 09/2010 to 09/2011 | **DAAD Annual Scholarship for Language Studies / Huayu Enrichment Scholarship**<br>National Sun Yat-Sen University, Kaohsiung, Taiwan |
| | Full-time Chinese language studies. |
| 09/2009 to 06/2010 | **ERASMUS Exchange**<br>Dept. of Physics, Vrije Universiteit Amsterdam, Netherlands |
| 09/2000 to 06/2007 | **A-Level** (grade 1.3)<br>Campe Gymnasium Holzminden, Germany |
| | Foci: Mathematics, Latin, Physics, Politics |

## Professional Experience

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| since 10/2025 | **Specially Appointed Assistant Professor**<br>Department of Complex Systems Science, Graduate School of Informatics, Nagoya University, Japan |
| 08/2021 to 09/2025 | **Data Steward** (part-time)<br>*liv*MatS Cluster of Excellence, University of Freiburg, Germany<br><br>Lead policy development for digital transformation. Developed and maintained dtool & dserver data management ecosystem. |
| 05/2022 to 09/2023 | **Co-founder, CTO** (part-time)<br>Start Up *Surface Design Solutions*<br><br>Applied machine learning methods (GPC, GPR) to predict performance of surface finish based on topography data. |
| 02/2017 to 09/2023 | **Examiner** (repeated assignments of two to four months each)<br>Academic Evaluation Center, a joint institution of the German Embassy's cultural department and the German Academic Exchange Service (DAAD)<br><br>Conducted interviews for plausibility verification of academic records. |
| 01/2021 to 07/2021 | **Parental Leave** |
| 09/2014 to 06/2015 | **German Teacher** (part-time)<br>University-affiliated language courses at Beijing Language and Culture University and Peking University<br><br>Taught preparatory courses for academic studies in Germany. |
| 08/2007 to 07/2008 | **Working Holiday**<br>Australia<br><br>Various jobs in meat processing and hotel industry. |

## Journal Publications

Liu, C., **Hörmann, J. L.**, Pan, H., Xu, H., Han, L., Cheng, J., Chen, X., Zeng, H., Meng, Y., Tian, Y. *Friction-Assisted Electrochemical Oxidation of Iridium Surfaces for Enhanced Catalysis*. Mater. Horiz. 2026, ahead of print. https://doi.org/10.1039/D6MH00036C.

**Hörmann, J. L.**; Yanes, L.; Vazhappilly, A.; Sanner, A.; Holey, H.; Pastewka, L.; Hartley, M.; Olsson, T. S. G. *Dtool and Dserver: A Flexible Ecosystem for Findable Data*. PLOS ONE 2024, 19 (6), e0306100. https://doi.org/10.1371/journal.pone.0306100.

Grigorev, P.; Frérot, L.; Birks, F.; Gola, A.; Golebiowski, J.; Grießer, J.; **Hörmann, J. L.**; Klemenz, A.; Moras, G.; Nöhring, W. G.; Oldenstaedt, J. A.; Patel, P.; Reichenbach, T.; Rocke, T.; Shenoy, L.; Walter, M.; Wengert, S.; Zhang, L.; Kermode, J. R.; Pastewka, L. *Matscipy: Materials Science at the Atomic Scale with Python*. Journal of Open Source Software 2024, 9 (93), 5668. https://doi.org/10.21105/joss.05668.

**Hörmann, J. L.**; Liu, C. (刘宸旭); Meng, Y. (孟永钢); Pastewka, L. *Molecular Simulations of Sliding on SDS Surfactant Films*. J. Chem. Phys. 2023, 158 (24), 244703. https://doi.org/10.1063/5.0153397.

Seidl, C.; **Hörmann, J. L.**; Pastewka, L. *Molecular Simulations of Electrotunable Lubrication: Viscosity and Wall Slip in Aqueous Electrolytes*. Tribol Lett 2021, 69 (1), 22. https://doi.org/10.1007/s11249-020-01395-6.

## Proceedings Publications

**Hörmann, J. L.** & Pastewka, L. Lightweight research data management with dtool: a use case. in Proceedings of the 7th bwHPC Symposium vol. 7 29–35 (Universität Ulm, 2022).

**Hörmann, J. L.** & Pastewka, L. SDS adsorptions films at the H2O – Au(111) interface: molecular dynamics study of AFM tip–surface contact. in NIC Series vol. 50 101–107 (Forschungszentrum Jülich, Jülich, Germany, 2020).

## Conferences and select presentations

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| 09/2024 | ASIATRIB2024 & CICT2024: 7th Asia International Conference on Tribology & 9th China International Conference on Tribology, Tianjin, China. Oral presentation: *Reproducible molecular simulations of sliding on SDS surfactant films with dtool and dserver, a flexible ecosystem for distributed data management*. |
| 06/2024 | 9th European Nanomanipulation Workshop, Madrid, Spain. Oral presentation: *Sliding on SDS surfactant films -- molecular simulations*. |
| 06/2024 | ECCOMAS 2024: European Community on Computational Methods in Applied Sciences Congress 2024, Lisboa, Portugal. Oral presentation: *dtool and dserver: A flexible ecosystem for findable data*. |
| 09/2023 | ITC 2023: 9th International Tribology Conference, Fukuoka, Japan. Oral presentation: *Molecular simulations of sliding on SDS surfactant films.* |
| 03/2023 | LMS 2023: 1st International Conference and Scientific Exhibition on Living Materials Systems, Freiburg, Germany. Oral presentation: *Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics*. |
| 10/2022 | Data Stewardship Goes Germany 2022, Braunschweig, Germany. Oral presentation: *livMatS Research Data Management Concept with a focus on the didactic use of dtool*. |
| 10/2022 | MMM 2022: 10th Conference on Multiscale Materials Modeling, Baltimore, USA. Oral presentation: *Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics*. |
| 07/2022 | WTC 2022: 7th World Tribology Congress, Lyon, France. Oral presentation: *Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics.* |
| 09/2021 | 116th AGEF Symposium on Triboelectrochemistry, Bonn, Germany. Oral presentation. |
| 09/2019 | 46th Leeds-Lyon Symposium on Tribology, Lyon, France. Oral presentation. |
| 10/2018 | 9th Conference on Multiscale Materials Modeling, Osaka, Japan. Oral presentation. |
| 10/2018 | Beilstein Nanotechnology Symposium 2018, Molecular Mechanisms in Tribology, Potsdam, Germany. Poster presentation. |
| 09/2017 | WTC 2017: 6th World Tribology Congress, Beijing, China. Poster presentation. |

## Awards and Funding

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| 04/2026 | **Fugaku Junior Researchers (Small-Scale) Project: The influence of molecular design on tribological performance on the nanoscale**<br>Principal Investigator. Awarded 432,000 node-h computing time on HPC system Fugaku at Riken Center for Computational Science in Kobe, Japan. |
| 04/2026 | **NINS RCCS Category A Project: Sequence-Dependent Friction of Adsorbed Polymers: A Molecular Dynamics Study of Polyalkylmethacrylate Lubricant Additives**<br>Principal Investigator. Awarded 80,000 core points computing time on HPC system at Research Center for Computational Science (RCCS), Okazaki Common Research Facility, National Institutes of Natural Sciences (NINS), Japan. |
| 12/2025 | **Joint Research Advancement Program 2026-2027**<br>**University of Freiburg and Nagoya University**<br>Co-author of funding-winning joint proposal. |
| 09/2022 | **KTUR Summer School Entrepreneurship: Best Project Award**<br>Leader of award-winning team *surfAIce*. |
| 05/2021 to 04/2022 | **GCS/NIC Regular Project hfr21**<br>Awarded 3.36 mio core-h computing time on HPC system JUWELS at the Jülich Supercomputing Center (JSC), Germany. |
| 05/2020 to 04/2021 | **GCS/NIC Regular Project hfr13**<br>Awarded 3.4 mio core-h computing time on HPC system JUWELS at JSC. |
| 05/2019 to 04/2020 | **GCS/NIC Regular Project hfr13**<br>Awarded 2.2 mio core-h computing time on HPC system JUWELS at JSC. |
| 05/2018 to 04/2019 | **GCS/NIC Regular Project hfr13**<br>Awarded 2.6 mio core-h computing time on HPC system JUWELS at JSC. |
| 09/2017 | **6$^{th}$ World Tribology Congress, Beijing: Best Poster Award** |
| 09/2013 to 08/2014 | **DAAD Annual Scholarship for Exchange Studies**<br>Tsinghua University, Beijing, China. |
| 09/2010 to 09/2011 | **DAAD Annual Scholarship for Language Studies / Huayu Enrichment Scholarship**<br>National Sun Yat-Sen University, Kaohsiung, Taiwan. |

## Supervision experience

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| 01/2025 | Co-supervised Bachelor thesis: *Microfluidic elements* |
| 09/2024 | Co-supervised Bachelor thesis: *Influence of electrode roughness on the ion concentration in electrochemical double layers: Finite element simulations in two dimensions* |
| 01/2022 - 09/2025 | Supervision of various research assistants working on the *dtool & dserver* research data management ecosystem |
| 09/2021 | Co-supervised Bachelor thesis: *Finite element simulations of the electrochemical double layer structure under microscopic probes of various geometries* |
| 07/2020 | Co-supervised Master thesis: *Pressure and Voltage Effects on Lubrication by an Aqueous Electrolyte — A Molecular Dynamics Study* |

## Teaching experience

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| 2021 - 2025 | Several hands-on workshops on research data management best practices |
| summer term 2020 | Tutor for lecture *Simulation* |
| winter term 19/20 | Tutor for lecture *Differential Equations* |
| summer term 2019 | Lecture on classical force fields for molecular dynamics |
| winter term 18/19 | Tutor for lecture *Differential Equations* |
| summer term 2018 | Tutor for lecture *Simulation* |

## References

**Professor Lars Pastewka** (Ph.D. supervisor)
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**Professor Valentin L. Popov** (Master co-supervisor, collaborator in DFG-funded project AWEARNESS)
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**Dr. Andreas Greiner** (Group leader, collaborator on delivering lectures and mentoring students)
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