## **Curriculum Vitae**

## Johannes Laurin Hörmann

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born on 29<sup>th</sup> June 1988 German



### Research highlights

Experienced research professional specializing in computational modeling for micro- and nanotribology and materials science. Key achievements include:

- Established continuum models of rough interfaces using FEM to study solvent concentration variations on rough surfaces.
- Developed atomistic models of surfactant adsorption films using MD for Ph.D. research.
- Applied machine learning (GPC, GPR) to predict rough surface performance in an entrepreneurial venture.
- Co-coordinated proposal writing for the DFG-funded 'AWEARNESS' project, employing DFT to study zinc phosphate glasses typically grown as films in tribo-induced decomposition reactions of ZDDP, a common additive in engine oils.
- All these modeling contributions have been made possible by rigid design of reproducible workflows with well-established Workflow Management Systems (WMS).
- Leading developer and maintainer for the *dtool* & *dserver* data management ecosystem, a community effort.

Currently serving as Data Steward at the Cluster of Excellence livMatS.

Education	
07/2017-02/2025	<b>Ph.D. Microsystems Engineering</b> Simulation, Dept. of Microsystems Engineering (IMTEK), University of Freiburg, Germany
	Dissertation: Friction of Adsorption Films with Reproducible Molecular Dynamics
09/2014 to 01/2017	Master Mechanical Engineering Tsinghua University, Beijing, China
	Double Degree Master Program between Tsinghua University and Technische Universität Berlin
	Master thesis (grade 1.3, German scale): Computational Modeling of Potential-Controlled Dodecyl Sulfate Ion Adsorption at the Aqueous and Non-aqueous SDS Solution – Stainless Steel Interface
09/2012 to 03/2017	Master Engineering Science (grade 1.6, German scale) Technische Universität Berlin, Germany
	Foci: Mechatronics, Numerics & Simulation
09/2008 to 09/2012	Bachelor Physics (grade 2.0, German scale) Freie Universität Berlin, Germany
	Bachelor thesis (grade 1.0, German scale):  Large Scale Parallel Simulation of EPR Lineshape Spectra

06/2007 **A-Level** (grade 1.3)

Campe Gymnasium Holzminden, Germany Foci: Mathematics, Latin, Physics, Politics

## **Professional Experience**

since 08/2021	Data Steward
	livMatS Cluster of Excellence, University of Freiburg, Germany
05/2022 to 09/2023	Co-founder
	Start Up Surface Design Solutions
01/2021 to 2021/07	Parental Leave
since 02/2017	<b>Examiner</b> Academic examination office, a joint institution of the German Embassy's cultural department and the German Academic Exchange Service (DAAD)
since 02/2017	Academic examination office, a joint institution of the German Embassy's

#### **Journal Publications**

**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).

Awards and Funding	Awa	rds	and	Fun	ding
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09/2022	KTUR Summer School Entrepreneurship: Best Project Award
	Leader of award-winning team surfAlce
05/2021 to 04/2022	GCS/NIC Regular Project hfr21
	Awarded 3.36 mio core-h computing time on HPC system JUWELS at the Jülich Supercomputing Center (JSC)
05/2020 to 04/2021	GCS/NIC Regular Project hfr13
	Awarded 3.4 mio core-h computing time on HPC system JUWELS at JSC
05/2019 to 04/2020	GCS/NIC Regular Project hfr13
	Awarded 2.2 mio core-h computing time on HPC system JUWELS at JSC
05/2018 to 04/2019	GCS/NIC Regular Project hfr13
	Awarded 2.6 mio core-h computing time on HPC system JUWELS at JSC
09/2017	6 <sup>th</sup> World Tribology Congress, Beijing: Best Poster Award
09/2013 to 08/2014	<b>DAAD Annual Scholarship for Exchange Studies</b> Tsinghua University, Beijing, China
09/2010 to 09/2011	DAAD Annual Scholarship for Language Studies / Huayu Enrichment Scholarship National Sun Yat-Sen University, Kaohsiung, Taiwan
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# **Supervision experience**

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
since 2022	Supervision of various research assistants working on the <i>dtool &amp; dserver</i> 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: <i>Pressure and Voltage Effects on Lubrication</i> by an Aqueous Electrolyte — A Molecular Dynamics Study

# **Teaching experience**

since 2021	Several hands-on workshops on research data management best practices
summer term 2020	Tutor for lecure 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

09/2024	ASIATRIB2024 & CICT2024: 7 <sup>th</sup> Asia International Conference on Tribology & 9 <sup>th</sup> 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	9 <sup>th</sup> European Nanomanipulation Workshop, Madrid, Spain. Oral presentation: <i>Sliding on SDS surfactant films molecular simulations</i> .
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: 9 <sup>th</sup> International Tribology Conference, Fukuoka, Japan. Oral presentation: <i>Molecular simulations of sliding on SDS surfactant films</i> .
03/2023	LMS 2023: 1 <sup>st</sup> International Conference and Scientific Exhibition on Living Materials Systems, Freiburg, Germany. Oral presentation: <i>Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics</i> .
10/2022	MMM 2022: 10 <sup>th</sup> Conference on Multiscale Materials Modeling, Baltimore, USA. Oral presentation: <i>Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics.</i>
07/2022	WTC 2022: 7 <sup>th</sup> World Tribology Congress, Lyon, France. Oral presentation: <i>Morphology, concentration, potential: Exploring tunable adsorption film friction with molecular dynamics.</i>
09/2021	116 <sup>th</sup> AGEF Symposium on Triboelectrochemistry, Bonn, Germany. Oral presentation.
09/2019	46 <sup>th</sup> Leeds-Lyon Symposium on Tribology, Lyon, France. Oral presentation.
10/2018	9 <sup>th</sup> 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: 6 <sup>th</sup> World Tribology Congress, Beijing, China. Poster presentation.

# Skills & Qualifications

Skills & Qualifications	
scientific 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 (GPR, GPC) with gpflow and sklearn
	Computational Workflow Management with FireWorks and snakemake
	Research Data Management with dtool & dserver
DevOps skills	Github CI/CD, OpenStack, Docker, Podman, Singularity, Make, CMake, EasyBuild, Imod, Slurm, MongoDB, SQL databases, Flask, REST API
other tech skills	Python, C/C++, tcl, Lua, MATLAB, Mathematica, LaTeX
languages	German native, English fluent, Chinese fluent
driver's license	motorbike, car
interests	swimming, hiking, running, dancing, reading, cooking