Curriculum Vitae

Johannes Laurin Hörmann

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born on 29th June 1988
German

Research Highlights

- Established **electrochemical models** of electrolytes at rough interfaces using the **Finite Elements Method (FEM)** for solving a system of **Poisson-Nernst-Planck equations** to study solvent concentration variations.
- Developed atomistic models of surfactant adsorption films using **Molecular Dynamics (MD)** for studying their friction behavior in Ph.D. project.
- Applied **machine learning methods (GPC, GPR)** to predict rough surface performance in an entrepreneurial venture.
- Co-coordinated proposal writing for the DFG-funded 'AWEARNESS' project, employing **density functional theory (DFT)** to study zinc phosphate glasses typically grown as films in tribo-induced decomposition reactions of ZDDP, a common additive in engine oils.
- Designed **reproducible computational workflows** with well-established Workflow Management Systems (WMS).
- Co-developed and maintained the **open source dtool & dserver** data management ecosystem, a community effort.

Skills & Qualifications

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

07/2017 to 07/2025	**Ph.D. Microsystems Engineering** Simulation, Dept. of Microsystems Engineering (IMTEK), University of Freiburg, Germany Dissertation (https://doi.org/10.6094/UNIFR/269291): *Friction of Adsorption Films with Reproducible Molecular Dynamics*

09/2014 to 01/2017	**Master Mechanical Engineering** (Double Degree Master Program) Dept. of Mechanical Engineering, Tsinghua University, Beijing, China Master thesis (grade 1.3, German scale): *Computational Multiscale Modeling of the Bipolar Electrochemical Process*
09/2012 to 03/2017	**Master Engineering Science** (grade 1.6, German scale) 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) Dept. of Physics, Freie Universität Berlin, Germany Bachelor thesis (grade 1.0, German scale): *Large Scale Parallel Simulation of EPR Lineshape Spectra*
09/2010 to 09/2011	**DAAD Annual Scholarship for Language Studies / Huayu Enrichment Scholarship** National Sun Yat-Sen University, Kaohsiung, Taiwan Full-time Chinese language studies.
09/2009 to 06/2010	**ERASMUS Exchange** Dept. of Physics, Vrije Universiteit Amsterdam, Netherlands
09/2000 to 06/2007	**A-Level** (grade 1.3) Campe Gymnasium Holzminden, Germany Foci: Mathematics, Latin, Physics, Politics

Professional Experience

since 08/2021	**Data Steward** (part-time) *liv*MatS Cluster of Excellence, University of Freiburg, Germany Lead policy development for digital transformation. Developed and maintained dtool & dserver data management ecosystem.
05/2022 to 09/2023	**Co-founder, CTO** (part-time) Start Up *Surface Design Solutions* 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) Academic Evaluation Center, a joint institution of the German Embassy's cultural department and the German Academic Exchange Service (DAAD) Conducted interviews for plausibility verification of academic records.
01/2021 to 07/2021	**Parental Leave**
09/2014 to 06/2015	**German Teacher** (part-time) University-affiliated language courses at Beijing Language and Culture University and Peking University Taught preparatory courses for academic studies in Germany.
08/2007 to 07/2008	**Working Holiday** Australia Various jobs in meat processing and hotel industry.

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).

Conferences and select presentations

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

09/2022	**KTUR Summer School Entrepreneurship: Best Project Award**
	Leader of award-winning team *surfAIce*
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	**6th World Tribology Congress, Beijing: Best Poster Award**
09/2013 to 08/2014	**DAAD Annual Scholarship for Exchange Studies** 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

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 01/2022	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

since 2021	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*