Wojciech G. Stark

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Education

University of Warwick **Coventry, United Kingdom**
PhD in Computational Chemistry *Jun 2020 - May 2024*

- **Thesis:** "Machine learning models for gas-surface dynamics". [link]
- **Overview of the research:** Investigating dynamics of the hydrogen molecule at metal surfaces. Developing adaptive sampling (active learning) workflows to construct accurate and efficient machine learning interatomic potentials and machine learning models for studying nonadiabatic effects.
- **Supervisors:** Prof. Reinhard J. Maurer, Prof. Scott Habershon.

Warsaw University of Technology **Warsaw, Poland**
MSc in Chemical Technology and Catalysis *Feb 2017 - Dec 2018*

- **Thesis:** "Software for computer-aided design of experiments".
- **Overview of the research:** Developing a *C#*-based program for planning, optimisation, and analysis of chemical reactions (Do-Exp [link]). Optimisation of the hydrogen transfer reaction between furfural and isopropyl alcohol.
- **Supervisor:** Dr Piotr Winiarek.

BSc in Chemical Technology *Oct 2012 - Feb 2016*

- **Thesis:** "Computer program for creating Sankey diagrams".
- **Supervisor:** Dr Piotr Winiarek.
- **Side project (The Lewinski group):** Synthesis of organometallic compounds with the use of a Schlenk line (reactions with diethylzinc and various ligands).

Experience

Imperial College London **London, United Kingdom**
Research Associate in AI for Chemistry *Jan 2025 - now*

- Deploying multi-objective batch Bayesian optimisation workflows to accelerate the identification of new catalysts and reaction conditions for CO_2 capture.
- Designing machine learning models to predict physicochemical properties of Metal-Organic Frameworks (MOFs) and Ionic Liquids.
- Developing a robust Python library that integrates these AI tools.

University of Warwick **Coventry, United Kingdom**
Research Assistant/Fellow *Apr 2024 - Dec 2024*

- Developed automated tools for generating actively learned machine learning interatomic potentials to model gas-surface dynamics.
- Improved the efficiency of adaptive sampling procedures by implementing novel foundation models, reducing computational cost.
- Integrated an electronic friction tensor model with the MACE graph neural network architecture.
- Investigated hydrogen scattering and desorption dynamics on metal surfaces, assessing the impact of nonadiabatic effects.

Travelist.pl **Warsaw, Poland**
Junior Business Analyst / Business Analyst / Business Process Analyst *May 2017 - May 2020*

- Automated and optimised 15+ business processes using custom bots and scripts, saving over 250 hours of manual work per week.
- Designed a new data warehouse from multiple separate MySQL/PostgreSQL databases, enabling unified reporting.
- Delivered data-driven recommendations to the sales team based on trend analysis, directly influencing account management strategies.

ONICO OIL **Warsaw, Poland**
Intern / Data Analysis *Jan 2017 - April 2017*

- Analysed sales data, and developed automated reporting tools.

IMEC (INTER UNIVERSITY MICROELECTRONICS CENTRE) **Leuven, Belgium**
Intern in R&D Department *Mar 2016 - Nov 2016*

- Optimized wet and dry silicon etching processes at a semiconductor R&D fabrication site.
- Developed VBA-based tools to automate the analysis of etching data for functionalised monocrystalline silicon wafers.

Mały Inżynier (en. The Little Engineer) **Warsaw, Poland**
Instructor *Feb 2015 - Feb 2016*

- Facilitated science, engineering, and robotics workshops, including performing live chemical demonstrations.

MDM NT. **Bielsko-Biała, Poland**
Intern in Quality Control Department *Jul 2014*

- Conducted quality control testing on vapor-permeable PE/PP films for construction applications.

Publication list

2025 "Nonadiabatic reactive scattering of hydrogen on different surface facets of copper", W. G. Stark, C. L. Box, M. Sachs, N. Hertl, and R. J. Maurer, **Phys. Rev. B** 112, 3. [link]

2025 "Machine learning and data-driven methods in computational surface and interface science", L. Hoermann, W. G. Stark, and R. J. Maurer, **npj Comput. Mater.** 11, 1. [link]

2025 "Fine-tuning foundation models of materials interatomic potentials with frozen transfer learning", M. Radova, W. G. Stark, C. S. Allen, R. J. Maurer and A. P. Bartók, **npj Comput. Mater.** 11, 237. [link]

2025 "Machine learning configuration-dependent friction tensors in Langevin heatbaths", M. Sachs, W. G. Stark, R. J. Maurer and C. Ortner, **Mach. Learn.: Sci. Technol.** 6, 1, 015016. [link]

2024 "Room temperature hydrogen atom scattering experiments are not a sufficient benchmark to validate electronic friction theory", C. L. Box, N. Hertl, W. G. Stark and R. J. Maurer, **J. Phys. Chem. Lett.** 15, 51, 12520–12525. [link]

2024 "Benchmarking of machine learning interatomic potentials for reactive hydrogen dynamics at metal surfaces", W. G. Stark, C. van der Oord, I. Batatia, Y. Zhang, B. Jiang, G. Csányi, and R. J. Maurer, **Mach. Learn.: Sci. Technol.** 5, 3, 030501. [link]

2023 "Machine learning interatomic potentials for reactive hydrogen dynamics at metal surfaces based on iterative refinement of reaction probabilities", W. G. Stark, J. Westermayr, O. A. Douglas-Gallardo, J. Gardner, S. Habershon, and R. J. Maurer, **J. Phys. Chem. C** 127, 50, 24168–24182. [link]

2023 "Ab initio calculation of electron-phonon linewidths and molecular dynamics with electronic friction at metal surfaces with numeric atom-centred orbitals", C. L. Box, W. G. Stark and R. J. Maurer, **Electron. Struct.** 5, 035005. [link]

2022 "NQCDynamics.jl: A Julia package for nonadiabatic quantum classical molecular dynamics in the condensed phase", J. Gardner, O. A. Douglas-Gallardo, W. G. Stark, J. Westermayr, S. M. Janke, S. Habershon and R. J. Maurer, **J. Chem. Phys.** 156, 174801. [link]

Scientific Talks

2025 **Psi-k conference (as a nominee for the Collaborating Early-Career Investigators award)**, Lausanne, Switzerland (*Invited*).
2023 **FHI-aims Developers' and Users' Meeting**, Hamburg, Germany (*Invited*).
2023 **GAP/(M)ACE Developers' and Users' Meeting**, Coventry, UK (*Contributed*).
2023 **Gordon Research Seminar** (Dynamics at Surfaces), Newport, RI, USA (*Contributed*).
2023 **M3S** (Multiscale Modelling of Materials and Surfaces) conference, Ambleside, UK (*Contributed*).
2023 **Faraday Joint Interest Group** conference, Sheffield, UK (*Contributed*).
2023 **DPG** (German Physical Society) Spring Meeting of the Condensed Matter Section, Dresden, Germany (*Contributed*).
2023 **APS** (American Physical Society) March Meeting, Las Vegas, NV, USA (*Contributed*).
2022 **ACS** (American Chemical Society) Spring Meeting, San Diego, CA, USA (*Contributed*).
2022 **DQML** (Dynamics, Quantum Effects, and Machine Learning in Materials Science and Computational Chemistry) conference, Lux, Austria (*Contributed*).

Poster Presentations

2023 **GRC** (Gordon Research Conference), Dynamics at Surfaces, Salve Regina University, Newport, RI, USA.
2022 **DPG** (German Physical Society) Spring Meeting of the Condensed Matter Section, Regensburg, Germany.
2022 **Psi-k** conference, SwissTech Convention Center, EPFL, Lausanne, Switzerland.
2022 **ML4M** Young Researcher's Workshop on Machine Learning for Materials, Trieste, Italy.
2022 **Supercomputer modelling of advanced materials** meeting, London, UK.
2022 **Postgraduate Research Symposium** University of Warwick, Coventry, UK.

Fellowships/Awards

2025 Runner-up to the **Psi-k Collaborating Early-Career Investigators (CECI) Award** (1 of 5 finalist teams), awarded for "exemplary scientific achievements realized in, and thanks to, the essential collaboration of a team of two or more early-career investigators" (Lausanne, Switzerland).
2012/2014 Recipient of **National Centre for Research and Development merit scholarship** (2 times), Warsaw University of Technology.

Professional Skills

Technical:	Python (*Advanced*)	Julia (*Intermediate/Advanced*)
	VBA (*Advanced*)	*C#* (*Intermediate*)
	PyTorch	SQL
	GitHub/GitLab	LaTeX
	FHI-aims	Quantum Espresso
Languages:	English (*Full professional proficiency*)	Polish (*Native*)
	Italian (*Beginner*)	