Mike **Pols**

PhD Candidate - Computational Materials Science - Eindhoven University of Technology, The Netherlands

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Leveraging extensive experience in training reactive and machine-learning force fields, I have investigated ion, phase, and lattice dynamics of halide perovskites. My goal is to advance machine-learning models beyond energy and force predictions to also cover charges, electronic structure, and spin properties, enabling applications in catalysis, optoelectronics, and spintronics.

Research Experience

Eindhoven University of Technology (TU/e)

Eindhoven, NL

PhD (Cum laude) in Materials Simulation & Modelling (MSM) *Mar. 2021 - Feb. 2025*

Computational modelling of halide perovskites using atomistic simulations, with a focus on their ion, phase, and lattice dynamics.

MSc in Applied Physics (Cum laude), MSc in Chemical Engineering (Cum laude) *May. 2018 - Feb. 2021*

- Grade Point Average (GPA): 9.4/10
- Master thesis: A Reactive Force Field for Large Scale Simulations of Metal Halide Perovskites (9.5/10) [Pub. 7]
- Industrial internship at Software for Chemistry & Materials (SCM) on infrared and Raman spectroscopy in solids (9.5/10)
- Research assistant at TU/e investigating atom-thin 2D materials for perovskite solar cells using computational modelling [Pub. 18]

BSc in Applied Physics (Cum laude), BSc in Chemical Engineering (Cum laude) *Sep. 2014 - Apr. 2018*

- Grade Point Average (GPA): 9.3/10
- Bachelor thesis: Triplet-triplet annihilation of phosphorescent host-guest materials for OLEDs (9.5/10)
- Research assistant at TU/e investigating triplet-triplet annihilation in phosphorescent host-guest systems for OLEDs [Pub. 19]

Teaching & Mentoring

Courses

TU/e, NL

Advanced Materials Modelling using Multiscale Methods (3MQ110) *2021 - 2023*

- Design of the course materials, including programming exercises and introductory density functional theory simulations
- Teaching assistant for hands-on programming exercises for density functional theory
- General introduction to use of high-performance computing (HPC) systems
- Supervision of student projects using classical and quantum simulations of halide perovskites

Computational Materials Science (3MN200) *2019 - 2020*

- Teaching assistant for hands-on density functional theory calculations with VASP
- General introduction to use of high-performance computing (HPC) systems

Student Mentoring

Mentored a variety of students at various levels during their thesis and internship projects:

- Master students (5) with projects covering ion migration, surface and grain boundary stability, and crystallization of halide perovskites
- Bachelor student (1) with project focused at exploring the compositional effects on structural chirality in chiral perovskites

Honors & Awards

Jun. 2024	**Participant of 73rd Lindau Meeting**, Lindau Nobel Laureate Meetings	*Lindau, Germany*
Feb. 2023	**HPC SYSTEMs Inc. Poster Award**, APATCC-10	*Quy Nhon, Vietnam*
Nov. 2021	**Best Poster Prize**, ACOS conference 2021	*Eindhoven, NL*
Sep. 2021	**Nominated: Best Student Assistant (Applied Physics, TU/e)**, STOOR Education Awards	*Eindhoven, NL*
Jun. 2020	**Participant of 70th Lindau Meeting**, Lindau Nobel Laureate Meetings	*Lindau, Germany*
May. 2018	**ALSP Scholarship (top 1%)**, Eindhoven University of Technology (TU/e)	*Eindhoven, NL*
Jul. 2014	**Bronze Medal (128th out of 291)**, 46th International Chemistry Olympiad	*Hanoi, Vietnam*
Jun. 2014	**Gold Medal (4th out of 4090)**, Dutch National Chemistry Olympiad 2014	*Amsterdam, NL*

Skills

Languages	**Dutch**: native, **English**: full professional proficiency, **German**: elementary
Programming	Python, Matlab, Mathematica, Fortran, LaTeX
Software	VASP, AMS, Phonopy, OVITO, VESTA, LAMMPS

Publications

First-author publications

1. **M. Pols**, E. Boom, G. Brocks, S. Calero, and S. Tao, 'Lattice Dynamics of Chiral 2D Perovskites: Pb vs. Sn', In preparation (2024).

2. **M. Pols**, G. Brocks, S. Calero, and S. Tao, 'Chiral Phonons in 2D Halide Perovskites', arXiv:2411.17225 (2024), DOI: 10.48550/arXiv.2411.17225.

3. **M. Pols**, G. Brocks, S. Calero, and S. Tao, 'Temperature-Dependent Chirality in Halide Perovskites', *J. Phys. Chem. Lett.*, 15, 8057-8064 (2024), DOI: 10.1021/acs.jpclett.4c01629.

4. **M. Pols**, A.C.T. van Duin, S. Calero, and S. Tao, 'Mixing I and Br in Inorganic Perovskites: Atomistic Insights from Reactive Molecular Dynamics Simulations', *J. Phys. Chem. C*, 128, 4111-4118 (2024), DOI: 10.1021/acs.jpcc.4c00563.

5. **M. Pols**, V. Brouwers, S. Calero, and S. Tao, 'How Fast Do Defects Migrate in Halide Perovskites: Insights From On-the-Fly Machine-Learned Force Fields', *Chem. Commun.*, 59, 4660-4663 (2023), DOI: 10.1039/D3CC00953J.

6. **M. Pols**, T. Hilpert, I. Filot, A.C.T. van Duin, S. Calero, and S. Tao, 'What Happens at Surfaces and Grain Boundaries of Halide Perovskites: Insights from Reactive Molecular Dynamics Simulations of $CsPbI_3$', *ACS Appl. Mater. & Interfaces*, 14, 40841-40850 (2022), DOI: 10.1021/acsami.2c09239.

7. **M. Pols**, J.M. Vicent-Luna, I. Filot, A.C.T. van Duin, and S. Tao, 'Atomistic Insights Into the Degradation of Inorganic Halide Perovskite $CsPbI_3$: A Reactive Force Field Molecular Dynamics Study', *J. Phys. Chem. Lett.*, 12, 5519-5525 (2021), DOI: 10.1021/acs.jpclett.1c01192.

Collaborative publications

8. R. Nurdillayeva, R. Moral, **M. Pols**, D.-K. Lee, M.V. Altoe, C. Schwartz, S. Tao, and C.M. Sutter-Fella, 'Humidity Disrupts Structural and Chiroptical Properties of Chiral 2D Perovskites', Submitted (2024).

9. V. Tyagi, **M. Pols**, G. Brocks, and S. Tao, 'Tracing Ion Migration in Halide Perovskites with Machine Learned Force Fields', arXiv:2409.16051 (2024), DOI: 10.48550/arXiv.2409.16051.

10. S. Liu, **M. Pols**, X. Huang, Z. Huang, Z. Guo, L. Li, L. Wang, H. Dong, S. Tao, H. Zhou, L.-D. Sun, and C.-H. Yan, 'In-situ Polymerization Strategy for Blue Perovskite Light-Emitting Diodes with Ultra-high Efficiency Exceeding 20%', Under review (2024).

11. A.J. Chacón-García, H.G. Baldovi, **M. Pols**, S. Tao, S. Calero, S. Navalón, I.I. Vitorica-Yrezabal, A. Rodríguez-Diéguez, H. García, P. Horcajada, and Y. Pérez, 'Improving the Water Resistance of Bi-Based Perovskite-Inspired Materials for Vapor-Phase Photocatalytic Overall Water Splitting', *Solar RRL*, 8, 2400250 (2024), DOI: 10.1002/solr.202400250.

12. J. Liu, C. Zhu, **M. Pols**, Z. Zhang, F. Hu, L. Wang, C. Zhang, Z. Liu, S. Tao, M. Xiao, and X. Wang, 'Discrete Elemental Distributions Inside a Single Mixed-Halide Perovskite Nanocrystal for the Self-Assembly of Multiple Quantum-Light Sources', *Nano Lett.*, 23, 10089-10096 (2023), DOI: 10.1021/acs.nanolett.3c03761.

13. A.S. Mirza, **M. Pols**, W. Soltanpoor, S. Tao, G. Brocks, and M. Morales-Masis, 'The Role of Sulfur in Sulfur Doped Copper(I) Iodide p-type Transparent Conductors', *Matter*, 6, 1-15 (2023), DOI: 10.1016/j.matt.2023.10.003.

14. Z. Qin, **M. Pols**, M. Qin, J. Zhang, H. Yan, S. Tao, and X. Lu, 'Over-18%-Efficiency Quasi-2D Ruddlesden-Popper Pb-Sn Mixed Perovskite Solar Cells by Compositional Engineering', *ACS Energy Lett.*, 8, 3188-3195 (2023), DOI: 10.1021/acsenergylett.3c00853.

15. S. Raaijmakers, **M. Pols**, J.M. Vicent-Luna, and S. Tao, 'Refined GFN1-xTB Parameters for Engineering Phase-Stable $CsPbX_3$ Perovskites', *J. Phys. Chem. C*, 126, 9587-9596 (2022), DOI: 10.1021/acs.jpcc.2c02412.

16. C. Onwudinanti, **M. Pols**, G. Brocks, V. Koelman, A.C.T. van Duin, T. Morgan, and S. Tao, 'A ReaxFF Molecular Dynamics Study of Hydrogen Diffusion in Ruthenium–The Role of Grain Boundaries', *J. Phys. Chem. C*, 126, 5950-5959 (2022), DOI: 10.1021/acs.jpcc.1c08776.

17. H. Xie, Z. Wang, Z. Chen, C. Pereyra, **M. Pols**, K. Gałkowski, M. Anaya, S. Fu, X. Jia, P. Tang, D.J. Kubicki, A. Agarwalla, H.-S. Kim, D. Prochowicz, X. Borrisé, M. Bonn, C. Bao, X. Sun, S.M. Zakeeruddin, L. Emsley, J. Arbiol, F. Gao, F. Fu, H.I. Wang, K.-J. Tielrooij, S. Stranks, S. Tao, M. Grätzel, A. Hagfeldt, and M. Lira-Cantu, 'Decoupling the Effects of Defects on Efficiency and Stability Through Phosphonates in Stable Halide Perovskite Solar Cells', *Joule*, 5, 1246-1266 (2021), DOI: 10.1016/j.joule.2021.04.003.

18. Y. Sun, Y. Yin, **M. Pols**, J. Zhong, Z. Huang, B. Liu, J. Liu, W. Wang, H. Xie, G. Zhan, Z. Zhou, W. Zhang, P. Wang, C. Zha, X. Jiang, Y. Ruan, C. Zhu, G. Brocks, X. Wang, L. Wang, J. Wang, S. Tao, and W. Huang, 'Engineering the Phases and Heterostructures of Ultrathin Hybrid Perovskite Nanosheets', *Adv. Mater.*, 32, 2002392 (2020), DOI: 10.1002/adma.202002392.

19. A. Ligthart, X. de Vries, L. Zhang, **M. Pols**, P.A. Bobbert, H. van Eersel, and R. Coehoorn, 'Effect of Triplet Confinement on Triplet–Triplet Annihilation in Organic Phosphorescent Host–Guest Systems', *Adv. Func. Mater.*, 28, 1804618 (2018), DOI: 10.1002/adfm.201804618.

Other publications

20. **M. Pols**, 'Metal Halide Perovskites: Shimmering But Shaky', *N! (TU/e Applied Physics Faculty Magazine)*, 57, 20-23 (2024).

Presentations

NWO CHAINS 2024 — *Veldhoven, NL, Dec. 2024*
Talk: Structural and Dynamic Chirality in 2D Halide Perovskites

Elementary School Tour at Applied Physics @ TU/e — *Eindhoven, NL, Jun. 2024*
Lecture: What Does a Computational Scientist Do At TU/e?

KNCV-CTC 2024 — *Eindhoven, NL, Apr. 2024*
Talk: Stability of Metal Halide Perovskites: Insights from Multiscale Reactive Molecular Dynamics Simulations

NWO Physics 2024 — *Veldhoven, NL, Jan. 2024*
Talk: Structural Descriptors for Chiral Halide Perovskites at Finite Temperatures

IUPAC | CHAINS 2023 — *The Hague, NL, Aug. 2023*
Talk: Reactive Molecular Dynamics Simulations of Metal Halide Perovskites

Elementary School Tour at Applied Physics @ TU/e — *Eindhoven, NL, Jun. 2023*
Lecture: What Does a Computational Scientist Do At TU/e?

CCER Seminar (3rd Year) — *Eindhoven, NL, Apr. 2023*
Talk: Multiscale Modelling of Defects in Halide Perovskites: Insights from a Variety of Computational Methods

Asia Pacific Conference of Theoretical and Computational Chemistry (APATCC-10) — *Quy Nhon, Vietnam, Mar. 2023*
Talk: Reactive Molecular Dynamics Simulations of Defect-Induced Degradation in Halide Perovskites: Insights from Machine Learned Force Fields and ReaxFF

2022 MRS Fall Meeting — *Boston, United States, Nov. 2022*
Talk: Multiscale Modelling of Defects in Halide Perovskites — Implications for the Phase Stability and Degradation Reactions Induced by Thermochemical Stress

Computational Methods in Nanothermodynamics — *Trondheim, Norway, Apr. 2022*
Talk: Reactive Molecular Dynamics Simulations of Metal Halide Perovskites

Green Week Lunch Lecture — *Eindhoven, NL, Mar. 2022*
Talk: What can I do as a physicist in the field of sustainability within Materials Simulations & Modelling (MSM)?

Han-sur-Lesse Winterschool 2021 — *Han-sur-Lesse, Belgium, Dec. 2021*
Lecture: A Reactive Force Field for Large Scale Simulations of Metal Halide Perovskites

CCER Seminar (First year) — *Eindhoven, NL, Apr. 2021*
Talk: A Reactive Force Field for Large Scale Simulations of Metal Halide Perovskites

Posters

DuComS Day 2023 — *Utrecht, NL, Nov. 2023*
Poster: On-the-fly Machine Learned Force Fields for Halide Perovskites: How Fast Do Defects Move?

NWO Physics 2023 — *Veldhoven, NL, Apr. 2023*
Poster: On-the-fly Machine Learned Force Fields for Halide Perovskites: How Fast Do Defects Move?

Asia Pacific Conference of Theoretical and Computational Chemistry (APATCC-10) — *Quy Nhon, Vietnam, Feb. 2023*
Poster: What Happens at Surfaces and Grain Boundaries of Halide Perovskites: Insights from Reactive Molecular Dynamics Simulations of $CsPbI_3$ **(HPC SYSTEMs Inc. Poster Award)**

Next-Generation V+ PV Materials 2022 — *Groningen, NL, Jul. 2022*
Poster: Atomistic Insights Into the Stability of Inorganic $CsPbI_3$ from Reactive Molecular Dynamics: The Impact of Defects, Surfaces and Grain Boundaries

Physics@Veldhoven 2022 — *Online, Jan. 2022*
Poster: Atomistic Insights Into Degradation Pathways Of Inorganic Metal Halide Perovskites

Applied Computational Science (ACOS) conference 2021 *Eindhoven, NL*
Poster: Atomistic Insights Into the Degradation of Inorganic Halide Perovskite $CsPbI_3$ **(Best Poster Prize)** *Nov. 2021*

2020 Virtual MRS Spring/Fall Meeting & Exhibit *Online*
Poster: A Reactive Force Field for Large Scale Simulations of Metal Halide Perovskites *Nov. 2020*

Internet Conference on Theory and Computation of Halide Perovskites (ComPer) *Online*
Poster: A Reactive Force Field for Large Scale Simulations of Metal Halide Perovskites *Sep. 2020*