Matthias Kellner

Curriculum Vitae

Bussigny, Vaud, Switzerland

Google Scholar | ORCID | GitHub

Research Profile

I develop machine-learning methods for atomistic simulation, with a focus on uncertainty quantification. I am interested in determining when a model's predictions can be trusted and when they cannot, which is a question central to deploying ML reliably in the physical sciences. I am also involved in the development of universal machine learning potentials. I have developed the universal PET-MOLS model and applied it to study amorphously formulated active pharmaceutical ingredients. I also build deep-learning models for predicting NMR chemical shieldings, which I make available to the wider chemistry community.

Education

PhD, Materials Science 2023–present
EPFL Lausanne, labCOSMO Lausanne, Switzerland
Advisor: Prof. Michele Ceriotti.

M.Sc., Chemistry 2020–2022
Technical University of Munich Munich, Germany
Master's thesis: *Exploring multifidelity machine learning for chemical shift predictions*

B.Sc., Chemistry 2016–2020
Technical University of Darmstadt Darmstadt, Germany
Bachelor's thesis: *Following chemical reactions using dDNP NMR spectroscopy*

Research and Professional Experience

Doctoral Researcher 2023–present
EPFL Lausanne, labCOSMO (Group of Prof. Michele Ceriotti) Lausanne, Switzerland

- Develop uncertainty-quantification methods for machine-learning interatomic potentials
- Build deep-learning models for NMR chemical shieldings in molecular organic solids (ShiftML)
- Develop universal machine learning potentials for condensed organic matter (PET-MOLS)

Working Student 2019–2021
TU Darmstadt, Krewald group, in collaboration with Janssen Pharmaceutica Darmstadt, Germany

- Computational study of stereoselective C-glycosylation reactions.

Publications

Peer-reviewed & accepted

[1] Bigi, F., Abbott, J. W., Loche, P., Mazitov, A., Tisi, D., Langer, M. F., Goscinski, A., Pegolo, P., Chong, S., Goswami, R., Febrer, P., Chorna, S., **Kellner**, **M.**, Ceriotti, M. & Fraux, G. "Metatensor and metatomic: foundational libraries for interoperable atomistic machine learning". In: *The Journal of Chemical Physics* 164.6 (2026), p. 064113. DOI: 10.1063/5.0304911.

[2] How, W. B., Febrer, P., Chong, S., Mazitov, A., Bigi, F., **Kellner**, **M.**, Pozdnyakov, S. & Ceriotti, M. "A universal machine learning model for the electronic density of states". In: *Digital Discovery* 5.4 (2026), pp. 1635–1649. DOI: 10.1039/d5dd00557d.

[3] Schäfer, M., **Kellner**, **M.**, Kästner, J. & Ceriotti, M. "How to Train a Shallow Ensemble". In: *Journal of Chemical Theory and Computation* 22.10 (2026), pp. 4939–4950. DOI: 10.1021/acs.jctc.6c00310.

[4] Chong, S., Bigi, F., Grasselli, F., Loche, P., **Kellner**, **M.** & Ceriotti, M. "Prediction rigidities for data-driven chemistry". In: *Faraday Discussions* 256 (2025), pp. 322–344. DOI: 10.1039/d4fd00101j.

[5] **Kellner**, **M.**, Holmes, J. B., Rodriguez-Madrid, R., Viscosi, F., Zhang, Y., Emsley, L. & Ceriotti, M. "A deep learning model for chemical shieldings in molecular organic solids including anisotropy". In: *The Journal of Physical Chemistry Letters* 16.34 (2025), pp. 8714–8722. DOI: 10.1021/acs.jpclett.5c01819. †

[6] Mazitov, A., Bigi, F., **Kellner**, **M.**, Pegolo, P., Tisi, D., Fraux, G., Pozdnyakov, S., Loche, P. & Ceriotti, M. "PET-MAD as a lightweight universal interatomic potential for advanced materials modeling". In: *Nature Communications* 16.1 (2025), p. 10653. DOI: 10.1038/s41467-025-65662-7.

[7] Balodis, M., Rao, Y., Stevanato, G., **Kellner**, **M.**, Meibom, J., Negroni, M., Chmelka, B. F. & Emsley, L. "Observation of Transient Prenucleation Species of Calcium Carbonate by DNP-Enhanced NMR". In: *The Journal of Physical Chemistry Letters* 15.31 (2024), pp. 7954–7961. DOI: 10.1021/acs.jpclett.4c01588.

[8] **Kellner**, **M.** & Ceriotti, M. "Uncertainty quantification by direct propagation of shallow ensembles". In: *Machine Learning: Science and Technology* 5.3 (2024), p. 035006. DOI: 10.1088/2632-2153/ad594a. †

[9] Litman, Y., Kapil, V., Feldman, Y. M. Y., Tisi, D., Begušić, T., Fidanyan, K., Fraux, G., Higer, J., **Kellner**, **M.**, Li, T. E., Pós, E. S., Stocco, E., Trenins, G., Hirshberg, B., Rossi, M. & Ceriotti, M. "i-PI 3.0: A flexible and efficient framework for advanced atomistic simulations". In: *The Journal of Chemical Physics* 161.6 (2024), p. 062504. DOI: 10.1063/5.0215869.

Preprints & manuscripts under review

[10] **Kellner**, **M.**, Hansen, T., Bligaard, T., Jacobsen, K. W. & Ceriotti, M. "Errors that matter: Uncertainty-aware universal machine-learning potentials calibrated on experiments". Under review. 2026. arXiv: 2604.24607. †

[11] **Kellner**, **M.**, Rodriguez-Madrid, R., Holmes, J. B., Unzueta, P. A., Beran, G. J., Emsley, L. & Ceriotti, M. "Machine-Learned NMR Shieldings in Molecular Solids with Built-In Hybrid-Functional Molecular Corrections". Submitted. 2026. arXiv: 2608.21313. †

[12] **Kellner**, **M.**, Rodriguez-Madrid, R., Holmes, J. B., Principe, V. P., Emsley, L. & Ceriotti, M. "Quantum-corrected NMR crystallography at scale". Under review. 2026. arXiv: 2603.06236. †

† First-author publication.

Invited Talks

- **SIAM Conference on Mathematical Aspects of Materials Science** — *Uncertainty quantification by direct propagation of shallow ensembles.* Pittsburgh, 2024.
- **Machine Learning for NMR Crystallography Workshop, CCP-NC** — *Advancing chemical shielding predictions in organic solids.* Manchester, 2025.
- **CECAM Workshop on Uncertainty Quantification in Atomistic Modeling** — *Practical uncertainty quantification for atomistic simulations with last-layer ensembles.* Lausanne, 2025.
- **XXVI Swiss NMR Symposium** — *Quantum-corrected NMR crystallography at scale.* Lausanne, 2026.
- **PASC 2026** — *Minisymposium, Trustworthy MLIPs - End-to-End Uncertainty Quantification for Atomistic Machine Learning.* Bern, 2026.
- **CAMD DTU seminar** — *End-to-End Uncertainty Quantification for Atomistic Machine Learning.* Copenhagen, 2026.
- **CCP-NC Seminar** — *Overview of ShiftML, QNC-NMR and open questions.* Online, 2026.

Contributed Talks

- **Workshop on Uncertainty Quantification in Molecular Simulation, MPI Magdeburg** — *Uncertainty quantification by direct propagation of shallow ensembles.* 2024.
- **DPG Spring Meeting** — *Uncertainty quantification by direct propagation of shallow ensembles.* Berlin, 2024.
- **DPG Spring Meeting** — *Advancing chemical shielding predictions in organic solids.* Regensburg, 2025.
- **NMRlipids Database Hackathon** — *Chemical shielding predictions in organic solids and beyond.* Bergen, 2025.
- **DPG Spring Meeting** — *NMR crystallography at finite temperatures.* Dresden, 2026.

Additional Conference Participation

- AMLD — Applied Machine Learning Days, EPFL, 2022.
- CECAM Workshop on machine-learning collective variables, Lausanne, 2022.
- CECAM Workshop on Path Integral Molecular Dynamics, Tel Aviv, 2023.
- Psi-K 2025, Lausanne, 2025.
- Conference on Frontiers in Atomistic Simulations: From Physics to Chemistry and Biology, Trieste, 2025.

Teaching Experience

EPFL	MSE-211 Organic Chemistry Lab — 2023, 2024, 2025. Lab instructor (small-group teaching).
	MSE-305 Introduction to Atomic-Scale Modeling — 2024. Teaching assistant.
	MSE-421 Statistical Thermodynamics — 2025. Teaching assistant.
	ICTP–MARVEL summer school — 2026. Tutor.
TUM	Python programming for chemistry students — 2022. Tutor.

Supervision and Mentoring

I regularly supervise master's project students at labCOSMO for semester projects and summer internships.

Previously supervised students

- Enrico Palermo, EPFL.
- Yuxuan Zhang (formerly Hong Kong University; now University of Oxford)
  –co-author of the ShiftML3 publication.
- Aurélien Wohrer (formerly EPFL; now master's project at EMPA).
- Seiio Inoue (University of Tokyo)
  –co-author of the QNC-NMR publication.

Outreach, Service, and Reviewing

Industrial outreach	Merck Innovation Cup, 2022.
Student outreach	Journee des gymnasien, EPFL, 2025.
Reviewing	JCTC, 1 manuscript, 2024.
	Nature Communications, 1 manuscript, 2026.
	JCP, 1 manuscript, 2026.

Technical Skills

Machine learning	Developing atomistic machine-learning models in PyTorch and Python.
HPC & codes	Experience with HPC systems, electronic-structure codes (VASP, Quantum ESPRESSO, ORCA, FHI-aims), and molecular-dynamics engines (i-PI, LAMMPS).

Software and Web Projects

ShiftML	shiftml.org: a web app for the prediction of chemical shieldings for organic crystals; averages ~100 unique visitors per month who submit ~200 calculations.
PyPI package	Maintainer of the `shiftml` PyPI package, which distributes the ShiftML model (~370 downloads in the past month).

Languages and Personal Information

Languages	German: native; English: fluent; French: fluent.
Nationality	German.