PIERO GASPAROTTO, PHD

Quantum Software Engineer @ Microsoft Quantum

piero.gasparotto@gmail.com **Seattle, WA** **piero-gasparotto**

EXPERIENCE

Quantum Software Engineer

Quantum Applications, Microsoft Quantum

Oct 2023 – Present — Redmond, USA

I lead the development of end-to-end AI4Science solutions, lead technological developments at the interface between computational chemistry, quantum computing and cloud-native agentic workflows.

Principal ML Scientist

AI4Chemistry, Ro5

Mar 2023 – Oct 2023 — New York, USA

Drove development of Ro5's 3D structure-based drug design platform and co-authored a peer-reviewed paper introducing Hydrascreen, a novel ML model for predicting protein-ligand binding affinities

Software Scientist

Scientific IT, Paul Scherrer Institute

May 2021 – Oct 2023 — Villigen, CH

My work focused on developing and deploying machine-learning–based methods to provide real-time feedback during kHz serial X-ray protein crystallography experiments.

Postdoc

Empa – ***nanotech@surfaces Group***

Apr 2019 – Mar 2021 — Dübendorf, CH

Focused on ML Force Fields, enhanced-sampling workflows, super-hard alloys and modeling of surface-catalysis reactions.

Postdoc

University College London – ***ICE Group***

Apr 2018 – Mar 2019 — London, UK

Developed a novel machine-learning force field for carbon-based materials and studied glassy interfacial water properties.

PhD Researcher

EPFL – ***COSMO Group***

Oct 2013 – Mar 2018 — Lausanne, CH

My research focused on unsupervised learning and pattern recognition methods combined with molecular dynamics and enhanced sampling techniques, with application to liquids, proteins and molecular crystals.

SELECTED PUBLICATIONS

- QDK/Chemistry: A Modular Toolkit for Quantum Chemistry Applications *arXiv preprint arXiv:2601.15253* (2026)
- TORO Indexer: A PyTorch-Based Indexing Algorithm for Kilohertz Serial Crystallography *J. Appl. Cryst.* **57**(4) (2024)

Full list: Google Scholar

EDUCATION

Ph.D. Computational Modelling

EPFL

2013–2018 — Lausanne, CH

M.Sc. Materials Science

University of Padua

2009–2012 — Padova, IT

B.Sc. Materials Science

University of Padua

2006–2009 — Padova, IT

FUNDING

Torres-Quevedo Technological Transfer Grant (2019)
With Acellera Labs, for hybrid Quantum/ML approaches for modeling metallo-proteins (€98k)

HPC Compute Grants
Awarded 5 compute grants at CSCS and UKCP/MCC ($350k)

TECH SKILLS

Python | Scripting | Molecular Dynamics | Quantum Chemistry | CI/CD | MLOps | DevOps | HPC | Deep Learning | Cloud Computing | Distributed Systems | Scientific Software | Workflows Orchestration | Agentic AI | Customer-facing Applications

MANAGEMENT

Project Lead | Agile | Cross-functional Teams | Mentorship

CONTRIBUTOR

QDK/Chemistry — Microsoft Quantum Applications Toolkit
TORO-Indexer — A PyTorch indexer for SX crystallography
Hydrascreen — Protein-ligand binding affinities
PLUMED — Enhanced sampling for molecular dynamics
PAMM — Probabilistic analysis of molecular motifs

LANGUAGES

Italian
English
French