

# PIERO GASPAROTTO, PHD

Quantum Software Engineer @ Microsoft Quantum

@ piero.gasparotto@gmail.com

📍 Seattle, WA

👤 piero-gasparotto

## EXPERIENCE

### Quantum Software Engineer

Quantum Applications, Microsoft Quantum

⌚ Mar 2025 – Present

📍 Redmond, USA

I develop AI-driven solutions for end-to-end quantum chemistry workflows, lead customer-facing applications, and integrate agentic AI workflows in Microsoft Discovery.

### Senior ML Engineer

Azure Quantum Elements, Microsoft Quantum

⌚ Oct 2023 – Feb 2025

📍 New York, USA

Focused on machine-learning models for materials and molecular simulations, alongside the design and operation of scalable, customer-facing infrastructure and automated workflows for HPC and cloud environments.

### 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

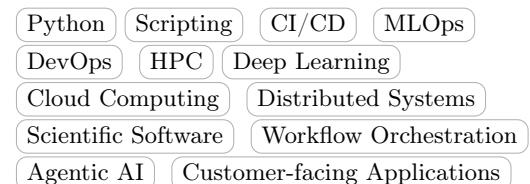
### 🏆 Torres-Quevedo Technological Transfer Grant (2019)

With Accelera 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



## MANAGEMENT



## 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

