

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

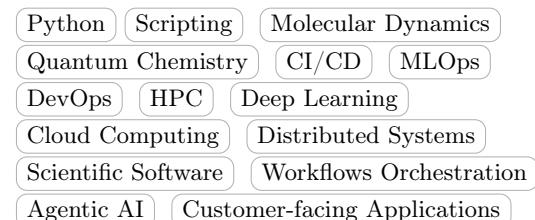
Torres-Quevedo Technological Transfer Grant (2019)

With 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

