Qi Shi, Ph.D.

Scientific Software Engineer · Imaging · Machine Learning
Lund, Sweden

qi2463sh@gmail.com

LinkedIn: linkedin.com/in/qi-shi-a26618171

GitHub: github.com/qi2463sh

Profile

Scientific software engineer with a Ph.D. in Chemical Physics and nearly a decade of experience developing **end-to-end imaging systems, machine-learning pipelines, and long-lived scientific software** at Lund University.
My work bridges **instrument control, data acquisition, modeling, and ML-based inference**, with a strong emphasis on **reliability, interpretability, and reproducibility**.
Experienced in translating complex experimental workflows into **maintainable software tools** used daily by collaborators across multi-year projects.

Core Skills

Scientific Software & Systems

- End-to-end pipeline design (acquisition → processing → modeling → visualization)
- Long-term maintainable research software (not one-off scripts)
- Instrument control, synchronization, and data acquisition
- Debugging complex hardware–software systems

Machine Learning & Data

- Supervised regression, CNNs (U-Net–style), ML for inverse problems
- Physics-informed modeling and validation
- Dataset curation, experiment tracking, evaluation (SSIM, MSE)
- Failure-mode analysis & model interpretability

Programming & Tools

- Python, MATLAB
- PyTorch, scikit-learn
- Scientific computing, signal processing
- HPC / GPU workflows (SLURM-based clusters)
- Git, Linux

Professional Experience

Postdoctoral Researcher — Scientific Software & Imaging

Lund University, Sweden
Jan 2021 – Dec 2025

- Designed and maintained a complete software stack for **intensity-modulated two-photon microscopy (IM-2PM)**, covering calibration, synchronized acquisition, data management, modeling, and ML-assisted analysis.
- Built **ML-assisted functional imaging pipelines** to extract spatially resolved physical parameters (trap states, recombination pathways) from nonlinear optical signals.
- Integrated **ODE-based physical simulations with supervised ML** to ensure interpretability and physical consistency.
- Developed **deep-learning super-resolution workflows** to enhance spatial resolution under photon budget and acquisition-time constraints.
- Deployed workflows on **GPU/HPC environments**, enabling scalable training and parameter inference.
- Produced stable tools used repeatedly by collaborators over multiple years.

Ph.D. Researcher — Nonlinear Optical Imaging & Data Analysis

Lund University, Sweden
Sep 2016 – Dec 2020

- Developed **intensity-modulated two-photon microscopy (IM-2PM)** for high-resolution mapping of charge-carrier dynamics in hybrid perovskites.
- Built analysis pipelines for **signal processing, model fitting, and parameter extraction**, transitioning from manual fitting to automated ML-based inference.
- Contributed to multi-institution collaborations combining spectroscopy, theory, and data-driven analysis.

Selected Projects (Engineering-Focused)

Instrument Control & Imaging Acquisition System (MATLAB GUI)

- Designed **MATLAB App Designer GUIs** for synchronized control of digitizers, piezo delay stages, and motorized translation stages.
- Implemented parameter validation and guardrails to prevent invalid hardware states.
- Enabled reliable, repeatable acquisition workflows used across PhD and postdoctoral experiments.

Technologies: MATLAB, GUI development, hardware APIs, data acquisition

AI-Enhanced Functional Imaging

- Built ML-assisted inference pipelines linking IM-2PM observables to physical recombination parameters.
- Combined ML predictions with ODE-based carrier population models.
- Enabled quantitative, spatially resolved mapping of trap-mediated losses.

Technologies: Python, ML regression, physical modeling, imaging pipelines

Energy & Environmental Materials (2025)

Deep Learning Super-Resolution for Functional Microscopy

- Developed CNN (U-Net–style) models for super-resolving functional IM-2PM maps.
- Designed training and validation strategies to avoid non-physical “hallucinated” features.
- Integrated inference into existing analysis workflows with standardized outputs and QC overlays.

Technologies: PyTorch, CNNs, SSIM/MSE evaluation, pipeline integration

ml-IM2PM: Machine Learning Regression for IM-2PM

- Implemented supervised regression models mapping modulation harmonics to physical parameters.
- Built a reproducible preprocessing, training, and validation pipeline.
- Replaced slow, fragile manual fitting with scalable ML inference.

ACS Photonics (2024)

LIBS + Machine Learning for Quantitative Elemental Analysis (M.Sc.)

- Applied SVR and PLSR to multi-element LIBS spectra.
- Compared univariate vs multivariate calibration strategies.
- Designed preprocessing and cross-validation workflows for robustness.

J. Anal. At. Spectrom. (2015, 2018); Analytical Methods (2019)

Education

- Undergraduate university:

Anyang Normal University, China, College of Chemistry and Chemical engineering, majoring in Chemical and Pharmaceutical, May 2013.

- Master university:

Sichuan University, China, Department of Chemistry, Analytical Chemistry, May 2016.
Thesis title: Exploration of Laser-induced Breakdown Spectroscopy (LIBS) in Quantitative Analysis of Sedimentary Rocks Based on Machine Learning.

- Ph.D. university:

Lund University, Sweden, Department of Chemistry, Division of Chemical Physics, Ph. D. defense December 2020. Advisor: Tönu Pullerits.
Thesis title: Phase modulation two photon microscopy of hybrid halide perovskite.

Grants & Awards

- Research grant from Fysiografiska 2018, Mapping the Spatial Distribuion of Large Polarons in Hybrid Perovskites Using Temperature Dependent Photoluminescence and Photocurrent Imaging

- Travel grant from Fysiografiska 2019, ICMAT 2019
- Light material profile Young Investigator Synergy Award 2023 with grant, Sustainable GaInP Nanowire based micro-LEDs (μ-LEDs) with AI-Enhanced Functional Imaging
- Travel grant from Lund University 2024, Nordic-Baltic Femtochemistry Conference 2024
- Light material profile Young Investigator Synergy Award 2025 with grant, Charge Dynamics in Lead-Free Perovskite Nanocrystals with Single-Atom Cocatalysts for CO_2 Photoreduction

Conferences, seminars, colloquia

Nanolund Annual meeting 2016-2024, Lund, posters.
Chemical Physics Science day 2016-2024, talk.
ICMAT 2019, Singapore, talk.
2nd LU-USTB, 2024, Invited speaker.
Nordic-Baltic Femtochemistry Conference 2024, talk.
LINXS Science Day on New Materials, 2024, poster.
Perovskite workshop 2023-2024, Lund, posters.
HAMLET-PHYSICS 2025 Conference, Copenhagen, talk.

Publications

13 selected articles out of over 26 per-reviewed journal publications, * marks the corresponding authors, citation data from Google Scholar, i10-index 20, h-index 16, total number of citations over 896 (2026/1/17).

Google Scholar link: https://scholar.google.com/citations?user=rlOFcsMAAAAJ&hl=en&oi=ao

1. Yukta, Rahman, S., **Shi, Q.**, Said, T.A., Matta, S.K., Hu, T., Wang, W., Opis-Basilio, A., Ray, K., Dick, K.A. and Pullerits, T., **2025**. M (III) Site-Driven Structural Engineering on Lead-Free Layered Double Perovskite Nanocrystals with Enhanced Photoelectrochemical Activity. *Small Structures*, p.2500179.

2. **Shi, Q***. and Pullerits, T*., **2025**. **AI**-Enhanced High-Resolution Functional Imaging Reveals Trap States and Charge Carrier Recombination Pathways in Perovskite. *Energy & Environmental Materials*, p.e70062. (1 citation)

3. **Shi, Q***. and Pullerits, T*., **2024**. **Machine Learning Regression Analyses** of Intensity Modulation Two-Photon Microscopy (ml-IM2PM) in Perovskite Microcrystals. *ACS Photonics,* 11(3), pp.1093-1102. (7 citation)

4. **Shi, Q.,** Kumar, P. and Pullerits, T*., **2023**. Temperature-Dependent Intensity Modulated Two-Photon Excited Fluorescence Microscopy for High Resolution Mapping of Charge Carrier Dynamics. *ACS Phys. Chem. Au.,* 3(5), pp.467-476. (5 citations)

5. Kumar, P., **Shi, Q.** and Karki, K.J*., **2019**. Enhanced radiative recombination of excitons and free charges due to local deformations in the band structure of MAPbBr3 perovskite crystals. *J. Phys. Chem. C., 123*(22), pp.13444-13450. (22 citations)

6. K. J. Karki, J. Chen, A. Sakurai, **Q. Shi,** A. T. Gardiner, O. Kühn, R. J. Cogdell, T. Pullerits*. **2019**. Before Förster. Initial excitation in photosynthetic light harvesting. *Chem. Science* 10, 7923. (64 citations)

7. Guo, G., Niu, G., **Shi, Q.,** Lin, Q., Tian, D. and Duan, Y*., **2019**. Multi-element quantitative analysis of soils by laser induced breakdown spectroscopy (LIBS) coupled with **univariate and multivariate regression methods**. *Analytical Methods*, *11*(23), pp.3006-3013. (103 citations)

8. **Shi, Q.,** Ghosh, S., Sarkar, A.S., Kumar, P., Wang, Z., Pal, S.K*., Pullerits, T*. and Karki, K.J*., **2018**. Variation in the photocurrent response due to different emissive states in methylammonium lead bromide perovskites. *J. Phys. Chem. C., 122*(7), pp.3818-3823. (14 citations)

9. **Shi, Q.,** Ghosh, S., Kumar, P., Folkers, L.C., Pal, S.K., Pullerits, T. and Karki, K.J*., **2018**. Variations in the composition of the phases lead to the differences in the optoelectronic properties of MAPbBr3 thin films and crystals. *J. Phys. Chem. C*, *122*(38), pp.21817-21823. (21 citations)

10. Niu, G., **Shi, Q.,** Yuan, X., Wang, J., Wang, X. and Duan, Y*., **2018**. Combination of **support vector regression (SVR)** and microwave plasma atomic emission spectrometry (MWP-AES) for quantitative elemental analysis in solid samples using the continuous direct solid sampling (CDSS) technique. *J. Anal. At. Spectrom.*, *33*(11), pp.1954-1961. (10 citations)

11. Ghosh, S., **Shi, Q.,** Pradhan, B., Kumar, P., Wang, Z., Acharya, S., Pal, S.K*., Pullerits, T*. and Karki, K.J*., **2018**. Phonon coupling with excitons and free carriers in formamidinium lead bromide perovskite nanocrystals. *J. Phys. Chem. Lett., 9*(15), pp.4245-4250. (79 citations)

12. **Shi, Q.,** Niu, G., Lin, Q., Xu, T., Li, F. and Duan, Y*., **2015**. Quantitative analysis of sedimentary rocks using laser-induced breakdown spectroscopy: comparison of **support vector regression and partial least squares regression chemometric methods**. *J. Anal. At. Spectrom.*, *30*(12), pp.2384-2393. (74 citations)

13. **Shi, Q.,** Niu, G., Lin, Q., Wang, X., Wang, J., Bian, F. and Duan, Y., **2014**. Exploration of a 3D nano-channel porous membrane material combined with laser-induced breakdown spectrometry for fast and sensitive heavy metal detection of solution samples. *Journal of analytical atomic spectrometry*, *29*(12), pp.2302-2308. (34 citations)