Christina Ertural

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in christina-ertural

R^G Christina-Ertural

◯ QuantumChemist

Nationality: German

Née Christina Zitlau

PROFILE

Software Developer with scientific background

I am a (scientific) Software Developer and Full Stack Quantum Chemist with extensive experience in building and maintaining complex software workflows in C++ and Python. Currently, I am also learning JavaScript/TypeScript and HTML/CSS. My expertise spans open source development, (quantum chemical) algorithms, data processing, high-performance computing, and creating user-facing cli tools. I bring strong problem-solving skills from academia and the ability to adapt quickly to new technologies.

PROFESSIONAL EXPERIENCE

2022 – 2025 — Postdoctoral Researcher (Software Development Focus in Materials Informatics)

BAM Federal Institute for Materials Research and Testing, Berlin (Governmental Research Institute)

- Designed and developed the Python workflow software AutoPLEX to automate large-scale data analysis and machine learning model generation, within the Materials Project software frameworks and based on MongoDB database management, resulting in scientific publications, 100+ stars on GitHub and a large user base.
- Created tools integrating machine learning models for material simulations.
- Collaborated in interdisciplinary teams, translating scientific needs into robust code.
- Applied modern open source software engineering practices (version control Git/GitHub, testing, documentation); working on tools like atomate2, pymatgen, jobflow-remote and qtoolkit, which have a huge user base.

2017 – 2022 — Software Developer / Doctoral thesis (Dr. rer. nat.)

RWTH Aachen University (Part of Germany's Excellence Initiative)

- C++ development and implementation of several quantum chemical bonding descriptors for the LOBSTER software (1k+ citations and huge user base) for electronic structure analysis, version control Apache Subversion SVN.
- Conducted computational research using VASP, Quantum ESPRESSO, ABINIT, resulting in publications with 2k+ citations.
- Supervised and trained students in quantum chemistry, coding and data analysis.

EDUCATION

2015 – 2017 — Master of Science, Chemistry
RWTH Aachen University

2011 – 2015 — Bachelor of Science, Chemistry
RWTH Aachen University

TECHNICAL SKILLS

Programming C++, Python, JavaScript/TypeScript, HTML/CSS, Git, GitHub, Linux, Bash scripting

Frameworks, Tools More MongoDB, PyTorch, TensorFlow, Node.js, Docker, HPC environments, Agile collaboration, Open Source Development, Machine Learning, Workshop Organization, Mentoring

LANGUAGES

German (native), English (fluent), French (intermediate)