Christina Ertural

✉ christina.ertural@quantumchemist.de

in christina-erural

R^G Christina-Ertural

○ QuantumChemist

Née Christina Zitlau, 30 January 1992 in Zavety Ilyicha, Russia
Nationality: German

CAREER

September 2022 – present

Postdoctoral Researcher

BAM Federal Institute for Materials Research and Testing in Germany
(Materials chemistry, Junior group George)

- Field of research: Materials Informatics, Development of software tools to enhance and accelerate *ab initio* calculations using automated workflows and machine-learned interatomic potentials
- Python workflow software development

ACADEMIC EDUCATION

December 2017 – July 2022

Doctoral degree (Dr. rer. nat.) in Chemistry

Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry,
RWTH Aachen University (Research group Dronskowski)

- Doctoral thesis: On the electronic structure of solid-state functional materials and their characterization using local bonding indicators (German)
- LOBSTER software development in C++ (cohp.de)

2015 – 2017

Master's degree in Chemistry

Department of Chemistry, RWTH Aachen University

- Master thesis: Quantum Monte Carlo-based Full Wave Function Optimization for Transition Metal Compounds (English)
  Institute of Physical Chemistry

2011 – 2017

Bachelor's degree in Chemistry

Department of Chemistry, RWTH Aachen University

- Bachelor thesis: Optimization of the Reaction Conditions for the Synthesis of Poly-Diacetylene Stabilized Gold Nanoparticles (German)
  Institute of Inorganic Chemistry

LANGUAGES

German (native), English (fluent)

FURTHER EXPERIENCE

Software and Coding Skills

- Languages: C++, Python, bash (Advanced)
- *Ab initio* software: LOBSTER (former developer), VASP (Advanced), Quantum ESPRESSO, ABINIT, Gaussian, Molpro (Basic)
- Graphic tools: Adobe Illustrator, CorelDRAW (Advanced)

Workshops

- HPC Tuning Workshop – Introduction to Performance Engineering and Analysis (aiXcelerate 2019)

Further skills

- Workshop and event organizing: LOBSTER schools, Berlin PostDoc Day 2023