Dr. Julian Geiger

Curriculum Vitae

General Information

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Residence 8458 Dorf, Zürich, Switzerland
Nationality German
Birth Date: 30th Nov 1994. Location: 90471 Nuremberg

Education

02/24 – 01/26 **Postdoctoral Researcher / Research Software Engineer** Paul-Scherrer Institute (PSI), Materials Software and Data Group of Dr. Giovanni Pizzi, Switzerland
02/23 – 05/23 **Research internship** EPFL, Nicola Marzari research group, Switzerland
10/19 – 10/23 **Chemistry PhD** Institute of Chemical Research of Catalonia (ICIQ), Núria López research group, Spain
06/18 – 12/18 **Master Thesis** BASF, Ansgar Schäfer research group (ROM/CQ), Germany, Grade: 1.0
10/17 – 03/18 **Erasmus semester** University of Cambridge, Michiel Sprik research group, UK
10/16 – 12/18 **Chemistry M.Sc.** Friedrich-Alexander-University Erlangen-Nuremberg (FAU), Germany, Grade: 1.0
04/16 – 07/16 **Bachelor thesis** FAU, Andreas Görling research group, Germany, Grade: 1.0
10/13 – 10/16 **Chemistry B.Sc.** FAU, Germany, Grade: 1.2
08/05 – 07/13 **A-levels** Adam-Kraft-Gymnasium Schwabach, Germany, Grade: 1.4

Work as a Research Software Engineer

`aiida-core` Contributor to and maintainer of the AiiDA workflow manager (large-scale project with >200k lines of Python code)

- ▷ Collaborative work in an intermediate-sized team (≈15 currently active members) on open-source, version-controlled software (using `git` and GitHub)
- ▷ General feature additions, usability improvements, bug fixes, and maintenance
- ▷ Focus on AiiDA's Object-Relational Mapper (ORM) implementation and data storage modules
- ▷ Implementation of a feature to extract data from AiiDA's SQL database (PostgreSQL / SQLite) and machine-readable disk-objectstore into human-readable directory trees (9k lines contribution)
- ▷ Familiarity with continuous integration (CI) tools such as pre-commit and GitHub Actions
- ▷ Experience with the full code quality infrastructure in place in AiiDA core: testing (pytest), linting (ruff), and static type checking (mypy)

`aiida-workgraph` Contributor to the AiiDA WorkGraph package to simplify dynamic workflow construction with AiiDA

- ▷ General API discussions, implementation of new features, documentation updates
- ▷ Integration of the CI pipeline used in AiiDA core into the AiiDA WorkGraph package

`sirocco` AiiDA-based Python workflow tool for weather & climate simulations

- ▷ Declarative, YAML-based workflow specification
- ▷ `pydantic` models for parsing and validation of workflow files
- ▷ `hatch` for Python project management

`renku integration` Integration of AiiDA and the renkulab.io platform for the exploration of AiiDA archives hosted on Materials Cloud Archive (MCA) using a containerized deployment

`basf/precomplex` Python and FORTRAN code for obtaining suitable input structures for automated transition-state searches for reaction path optimization algorithms (code in daily use in an industrial setting since 2018)

Honorable mentions
- ▷ Administrator of the group's High Performance Computing (HPC) cluster (10 nodes) using YAML configuration files to configure user accounts, SLURM, and a BeeGFS shared file system
- ▷ Supervision of Master student's semester project on optimizations to AiiDA's ORM layer and database interactions
- ▷ Responsible person for the AiiDA LinkedIn page and the publication of a blog post series
- ▷ Organization of regular AiiDA coding days and brainstorm meetings for team organization and planning
- ▷ Experience with various Quantum Chemistry simulation codes: VASP, Quantum ESPRESSO, CP2K, and Turbomole on HPC systems
- ▷ English proficiency (C2 level) and basic Spanish communication skills

Geeky stuff I like
- ▷ Currently learning the `rust` programming language
- ▷ Currently learning Apache Airflow in a team effort to replace AiiDA's internal engine by an industrial, general-purpose workflow manager
- ▷ Author of the AiiDA plugin for the `fish` shell (`plugin-aiida`)
- ▷ AstroNvim as IDE (with plugins, of course)
- ▷ `fish` shell with `tmux` as terminal environment
- ▷ Keyboard-driven `qutebrowser`

Scholarships

08/16 – 10/16 **DAAD RISE** 6-week chemistry internship at the Texas-Tech-University (Lubbock, USA)

2015 – 2018 **Deutschlandstipendium** funded by the German government and the Leonhard Kurz Stiftung & Co. KG

Conferences

13 – 14/08/2024 Hands-on workshop and panel discussion on FAIR Workflows in Materials Science (Purdue University, USA)

03 – 07/07/2023 IUVSTA-ZCAM: Metal-oxide ultrathin films and nanostructures: Experiment meets theory (Zaragoza, Spain): Poster contribution

22 – 25/08/2022 Psi-k conference (Lausanne, Switzerland): Poster contribution

Tutorials

13/08/2024 Hands-on session on AiiDA as part of the FAIR Workflows workshop (part 1 and part 2)

25/04/2024 Tutorial on shell configuration

29/06/2022 Introduction to VS Code

21/04/2021 Introduction to interactive visualization of scientific data with Plotly

Scientific Publications

2025 Janssen, J., George, J., **Geiger, J.** et al. A Python workflow definition for computational materials design. *arXiv preprint* arXiv:2505.20366.

2024 Minotaki, M., **Geiger, J.** et al., A generalized model for estimating adsorption energies of single atoms on doped carbon materials *J. Mater. Chem. A.* **18**, 2211260 (2024).

2023 Yang, Q., Surin, I., **Geiger, J.** et al. Lattice-Stabilized Chromium Atoms on Ceria for N_2O Synthesis. *ACS Catal.* **13**, 15977–15990 (2023).

2023 Surin, I., **Geiger, J.** et al., Low-Valent Manganese Atoms Stabilized on Ceria for Nitrous Oxide Synthesis. *Adv. Mater.* **35**, 2211260 (2023).

2022 **Geiger, J.**, Sabadell-Rendón, A., Daelman, N. et al. Data-driven models for ground and excited states for Single Atoms on Ceria. *npj Comput. Mater.* **8**, 171 (2022).

2022 **Geiger, J.** & López, N. Coupling Metal and Support Redox Terms in Single-Atom Catalysts. *J. Phys. Chem. C* **126**, 13698–13704 (2022).

2022 **Geiger, J.**, Settels, V., Deglmann, P. et al. Automated input structure generation for single-ended reaction path optimizations. *J. Comput. Chem.* **43**, 1662-1674 (2022).

2022 Wan, W., **Geiger, J.** et al. Highly Stable and Reactive Platinum Single Atoms on Oxygen Plasma-Functionalized CeO_2 Surfaces: Nanostructuring and Peroxo Effects. *Angew. Chem. Int. Ed.* **61**, e202112640 (2022).

2020 **Geiger, J.**, Sprik, M., May, M. M. et al. Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. *J. Chem. Phys.* **152**, 194706 (2020).