Julian Geiger

Curriculum Vitae

General Information

Birth	Date: 30th November 1994. Location: 90471 Nuremberg
Nationality	German
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Education

02/24 – present **Postdoc** *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
High-throughput study on the self-consistent evaluation of Hubbard U and V parameters of olivine and spinel Li-ion battery materials using Density Functional Perturbation Theory

10/19 – 10/23 **PhD** *Institute of Chemical Research of Catalonia, (ICIQ), Núria López research group*, Spain
Ceria-based Single-Atom Catalysts: From simplified models towards real world complexity

06/18 – 12/18 **Master Thesis** *BASF, Ansgar Schäfer research group (ROM/CQ)*, Germany, Grade: 1.0
Structure generation for the automated investigation of reaction networks using single-ended reaction path optimization algorithms

10/17 – 03/18 **Erasmus semester** *University of Cambridge, Michiel Sprik research group*, UK
Density Functional Theory study on the band alignment of anatase-TiO_2 surfaces in contact with water

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
Density Functional Theory investigations on potential catalysts for CO_2 activation on the basis of Cu(I)–NHC complexes with Turbomole

2013 – 2016 **Chemistry B.Sc.** *FAU, Germany*, Grade: 1.2

2005 – 2013 **A-levels** *Adam-Kraft-Gymnasium Schwabach*, Germany, Grade: 1.4

Scholarships

2015 – 2018 Financial funding by the German government and the Leonhard Kurz Stiftung & Co Kg through the German national scholarship program "Germany Scholarship"

08/16 – 10/16 6-week inorganic chemistry internship at the Texas-Tech-University, Lubbock (USA), funded by the "Research Internships in Science and Engineering" program of the German Academic Exchange Service (Daad Rise). *Michael Findlater research group*
Synthesis of Ir(I) – Pincer complexes and their usage as catalysts for the isomerization of internal alkynes to allenes

Conferences

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

22 – 25/08/2022 Psi-k conference (Poster contribution)

Skills

DFT codes	VASP, Quantum Espresso, CP2K, Turbomole
Programming	Python, Shell scripting (bash, fish), Fortran
Libraries	AiiDA, ASE, pymatgen, scikit-learn, pandas, plotly
Graphic design	Blender, Inkscape
Tools I love	VS Code, AstroNvim, git, fish shell, tmux, VIM keybindings, Obsidian
Soft skills	High degree of organization, driving scientific projects from conception to completion, independent work, effective communication in a team
Languages	German (native), English (C2), Spanish (B1)

Open source

`aiida-cattools`	Python utilities for the adaptation of AiiDA as a workflow engine in theoretical heterogeneous catalysis
`plugin-aiida`	AiiDA plugin for the fish shell
`sklwrap`	Wrapper functions for easy use and evaluation of sklearn predictors
`LopezGroup`	Maintainer of the Núria López group GitHub organization
`precomp_gen`	Precomplex generator: Tool for obtaining suitable input structures for automated transition-state (TS) searches with single-ended reaction path optimization algorithms (Master thesis project - Code in daily use in an industrial setting since 2018)

Tutorials

29/06/2022	Introduction to VS Code
21/04/2021	Introduction to interactive visualization of scientific data with Plotly

Publications

02/03/2023	Surin, I., **Geiger, J.** et al., Low-Valent Manganese Atoms Stabilized on Ceria for Nitrous Oxide Synthesis. *Adv. Mater.* **35**, 2211260 (2023).
18/08/2022	**Geiger, J.**, Sabadell-Rendón, A., Daelman, N. & López, N. Data-driven models for ground and excited states for Single Atoms on Ceria. *npj Comput. Mater.* **8**, 171 (2022).
05/08/2022	**Geiger, J.** & López, N. Coupling Metal and Support Redox Terms in Single-Atom Catalysts. *J. Phys. Chem. C* **126**, 13698–13704 (2022).
22/07/2022	**Geiger, J.**, Settels, V., Deglmann, P., Schäfer, A. & Bergeler, M. Automated input structure generation for single-ended reaction path optimizations. *J. Comput. Chem.* **43**, 1662-1674 (2022).
04/03/2022	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).
21/05/2020	**Geiger, J.**, Sprik, M. & May, M. M. Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. *J. Chem. Phys.* **152**, 194706 (2020).