



Julian Geiger

Curriculum Vitae

General

Current Location Institute of Chemical Research of Catalonia (ICIQ), 43007 Tarragona, Spain
Birth Date: 30th November 1994, 90471 Nuremberg
Nationality German
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Education

10/19 – present **PhD Student** *ICIQ, Núria López research group*
Investigations of ceria-based single-atom catalysts using Density Functional Theory, high-throughput simulations and machine learning
02/23 – 05/23 **Research internship** *EPFL, Nicola Marzari research group*
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
06/18 – 12/18 **Master Thesis** *BASF, Ansgar Schäfer research group (ROM/CQ)*, 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*
Hybrid Density Functional Theory study on the band alignment of anatase surfaces in contact with water
10/16 – 12/18 **Chemistry M.Sc.** *Friedrich-Alexander-University Erlangen-Nuremberg (FAU)*, Grade: 1.0
04/16 – 07/16 **Bachelor thesis** *FAU, Andreas Görling research group*, Grade: 1.0
Density Functional Theory investigations on potential catalysts for CO₂ activation on the basis of Cu(I)–NHC complexes with TURBOMOLE
2013 – 2016 **Chemistry B.Sc.** *FAU*, Grade: 1.2 (Valedictorian)
2005 – 2013 **A-levels** *Adam-Kraft-Gymnasium Schwabach*, 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). *Micheal 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 IUVESTA-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 CeO₂ 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).