



# 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  
E-Mail [jgeiger@iciq.es](mailto:jgeiger@iciq.es)

### Education

10/19 – present **PhD Student** *ICIQ, Núria López research group*  
Fundamental studies on 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*  
Density Functional Theory study on the band alignment of anatase-TiO<sub>2</sub> 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 CO<sub>2</sub> 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). *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 IUVESTA-ZCAM: Metal-oxide ultrathin films and nanostructures: Experiment meets theory (Poster contribution)  
22 – 25/08/2022 Psi-k conference (Poster contribution)






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## 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)

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## Open source

<code>aiida-cattools</code>	 Python utilities for the adaptation of AiiDA as a workflow engine in theoretical heterogeneous catalysis
<code>plugin-aiida</code>	 AiiDA plugin for the fish shell
<code>sklwrap</code>	 Wrapper functions for easy use and evaluation of sklearn predictors
<code>LopezGroup</code>	 Maintainer of the Núria López group GitHub organization
<code>precomp_gen</code>	 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)

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## Tutorials

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

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## Publications

02/03/2023	Surin, I., <b>Geiger, J.</b> et al., Low-Valent Manganese Atoms Stabilized on Ceria for Nitrous Oxide Synthesis. <i>Adv. Mater.</i> <b>35</b> , 2211260 (2023).
18/08/2022	<b>Geiger, J.</b> , Sabadell-Rendón, A., Daelman, N. & López, N. Data-driven models for ground and excited states for Single Atoms on Ceria. <i>npj Comput. Mater.</i> <b>8</b> , 171 (2022).
05/08/2022	<b>Geiger, J.</b> & López, N. Coupling Metal and Support Redox Terms in Single-Atom Catalysts. <i>J. Phys. Chem. C</i> <b>126</b> , 13698–13704 (2022).
22/07/2022	<b>Geiger, J.</b> , Settels, V., Deglmann, P., Schäfer, A. & Bergeler, M. Automated input structure generation for single-ended reaction path optimizations. <i>J. Comput. Chem.</i> <b>43</b> , 1662-1674 (2022).
04/03/2022	Wan, W., <b>Geiger, J.</b> et al. Highly Stable and Reactive Platinum Single Atoms on Oxygen Plasma-Functionalized CeO <sub>2</sub> Surfaces: Nanostructuring and Peroxo Effects. <i>Angew. Chem. Int. Ed.</i> <b>61</b> , e202112640 (2022).
21/05/2020	<b>Geiger, J.</b> , Sprik, M. & May, M. M. Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. <i>J. Chem. Phys.</i> <b>152</b> , 194706 (2020).