Julian Geiger

Curriculum Vitae

General

Current Location	43007 Tarragona, Spain
Birth	Date: 30th November 1994, 90471 Nuremberg
Nationality	German
E-Mail	jgeiger@iciq.es

Education

10/19 – present	**PhD Student** *Núria López research group*, Institute of Chemical Research of Catalonia
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
10/16 – 12/18	**Chemistry M.Sc.** *Friedrich-Alexander-University Erlangen-Nuremberg*, Grade: 1.0
04/16 – 07/16	**Bachelor thesis** *Andreas Görling research group*, 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.** *Friedrich-Alexander-University Erlangen-Nuremberg*, 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	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)

Workshops

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).