



# Julian Geiger

## Curriculum Vitae

### General Information

Address Avinguda dels Països Catalans 1, 43007 Tarragona, Spain  
Birth Date: 30th November 1994. Location: 90471 Nuremberg  
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### Education

10/19 – present **PhD Student** Núria López research group, Institute of Chemical Research of Catalonia  
06/18 – 12/18 **Master's 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's thesis** 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.** 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, funded by the “Research Internships in Science and Engineering” program of the German Academic Exchange Service (DAAD RISE). Findlater research group. Synthesis of Ir(I)–Pincer complexes and their usage as catalysts for the isomerization of internal alkynes to allenes.

### List of publications

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., Berdunov, N., Luna, M. L., Chee, S. W., Daelman, N., López, N., Shaikhutdinov, S. & Cuenya, B. R. Highly Stable and Reactive Platinum Single Atoms on Oxygen Plasma-Functionalized CeO<sub>2</sub> 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).