

# Florian GÃ¶ttl

## List of Publications by Year in descending order

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32  
papers

1,266  
citations

394421

19  
h-index

434195

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g-index

33  
all docs

33  
docs citations

33  
times ranked

1371  
citing authors

#	ARTICLE	IF	CITATIONS
1	Three Grand Challenges for the Computational Design of Heterogeneous Catalysts. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3305-3313.	3.1	7
2	Identifying hydroxylated copper dimers in SSZ-13 <i>via</i> UV-vis-NIR spectroscopy. <i>Catalysis Science and Technology</i> , 2022, 12, 2744-2748.	4.1	7
3	Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6079-6084.	4.6	8
4	Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13. <i>ACS Catalysis</i> , 2021, 11, 7719-7734.	11.2	31
5	Understanding Water-Zeolite Interactions: On the Accuracy of Density Functionals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20261-20274.	3.1	10
6	Diffusion Barriers for Carbon Monoxide on the Cu(001) Surface Using Many-Body Perturbation Theory and Various Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7862-7872.	5.3	10
7	Exploring driving forces for length growth in graphene nanoribbons during chemical vapor deposition of hydrocarbons on Ge(O $\alpha$ 1) <i>via</i> kinetic Monte Carlo simulations. <i>Applied Surface Science</i> , 2020, 527, 146784.	6.1	8
8	Computational description of key spectroscopic features of zeolite SSZ-13. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19065-19075.	2.8	11
9	Anisotropic Synthesis of Armchair Graphene Nanoribbon Arrays from Sub-5 nm Seeds at Variable Pitches on Germanium. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4266-4272.	4.6	17
10	Consequences of exchange-site heterogeneity and dynamics on the UV-visible spectrum of Cu-exchanged SSZ-13. <i>Chemical Science</i> , 2019, 10, 2373-2384.	7.4	80
11	UV-Vis and Photoluminescence Spectroscopy to Understand the Coordination of Cu Cations in the Zeolite SSZ-13. <i>Chemistry of Materials</i> , 2019, 31, 9582-9592.	6.7	19
12	Cooperative Role of Water Molecules during the Initial Stage of Water-Induced Zeolite Dealumination. <i>ACS Catalysis</i> , 2019, 9, 5119-5135.	11.2	53
13	Alignment of semiconducting graphene nanoribbons on vicinal Ge(001). <i>Nanoscale</i> , 2019, 11, 4864-4875.	5.6	26
14	Synthesis Gas Conversion over Rh-Mn-W <sub>x</sub> /C/SiO <sub>2</sub> Catalysts Prepared by Atomic Layer Deposition. <i>ACS Catalysis</i> , 2018, 8, 10707-10720.	11.2	17
15	Developing a Thermodynamic Model for the Interactions between Water and Cu in the Zeolite SSZ-13. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6160-6169.	3.1	25
16	Formation of [Cu <sub>2</sub> O <sub>2</sub> ] <sup>2+</sup> and [Cu <sub>2</sub> O] <sup>2+</sup> toward C-H Bond Activation in Cu-SSZ-13 and Cu-SSZ-39. <i>ACS Catalysis</i> , 2017, 7, 4291-4303.	11.2	195
17	Developing a Descriptor-Based Approach for CO and NO Adsorption Strength to Transition Metal Sites in Zeolites. <i>Chemistry of Materials</i> , 2017, 29, 6434-6444.	6.7	34
18	Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites. <i>ACS Catalysis</i> , 2016, 6, 8404-8409.	11.2	83

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19	The impact of finite temperature on the coordination of Cu cations in the zeolite SSZ-13. <i>Catalysis Today</i> , 2016, 267, 41-46.	4.4	33
20	Silica-Grafted SnIV Catalysts in Hydrogen-Transfer Reactions. <i>ChemCatChem</i> , 2015, 7, 3190-3190.	3.7	0
21	Verursacht Dynamik das komplexe Infrarotspektrum von NO an Kupfer(II)-Zentren in Zeolithen?. <i>Angewandte Chemie</i> , 2015, 127, 7910-7915.	2.0	8
22	Can Dynamics Be Responsible for the Complex Multipeak Infrared Spectra of NO Adsorbed to Copper(II) Sites in Zeolites?. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7799-7804.	13.8	39
23	Silica-Grafted Sn <sup>IV</sup> Catalysts in Hydrogen-Transfer Reactions. <i>ChemCatChem</i> , 2015, 7, 3270-3278.	3.7	24
24	Effect of Temperature on the Adsorption of Short Alkanes in the Zeolite SSZ-13: Adapting Adsorption Isotherms to Microporous Materials. <i>ACS Catalysis</i> , 2014, 4, 2351-2358.	11.2	32
25	Importance of a Nonlocal Description of Electron-Electron Interactions in Modeling the Dissociative Adsorption of H <sub>2</sub> on Cu(100). <i>Journal of Physical Chemistry C</i> , 2014, 118, 5374-5382.	3.1	19
26	What Makes Copper-Exchanged SSZ-13 Zeolite Efficient at Cleaning Car Exhaust Gases?. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2244-2249.	4.6	112
27	Modelling the adsorption of short alkanes in protonated chabazite: The impact of dispersion forces and temperature. <i>Microporous and Mesoporous Materials</i> , 2013, 166, 176-184.	4.4	44
28	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. III. Energetics and vibrational spectroscopy of adsorbates. <i>Journal of Chemical Physics</i> , 2012, 136, 064503.	3.0	52
29	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. I. Structure and energetics. <i>Journal of Chemical Physics</i> , 2012, 136, 064501.	3.0	58
30	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. II. Electronic structure and photoluminescence spectra. <i>Journal of Chemical Physics</i> , 2012, 136, 064502.	3.0	24
31	Van der Waals interactions between hydrocarbon molecules and zeolites: Periodic calculations at different levels of theory, from density functional theory to the random phase approximation and Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2012, 137, 114111.	3.0	123
32	Alkane adsorption in Na-exchanged chabazite: The influence of dispersion forces. <i>Journal of Chemical Physics</i> , 2011, 134, 064102.	3.0	57