Florian GÃ¶ltl

List of Publications by Year
in descending order

32	1,266	394421 19	434195 31
papers	citations	h-index	g-index

33	33	33	1371
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Formation of [Cu₂O₂]²⁺ and [Cu₂O]²⁺ toward Câ€“H Bond Activation in Cu-SSZ-13 and Cu-SSZ-39. ACS Catalysis, 2017, 7, 4291-4303.	11.2	195
2	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 MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 137, 114111.	3.0	123
3	What Makes Copper-Exchanged SSZ-13 Zeolite Efficient at Cleaning Car Exhaust Gases?. Journal of Physical Chemistry Letters, 2013, 4, 2244-2249.	4.6	112
4	Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites. ACS Catalysis, 2016, 6, 8404-8409.	11.2	83
5	Consequences of exchange-site heterogeneity and dynamics on the UV-visible spectrum of Cu-exchanged SSZ-13. Chemical Science, 2019, 10, 2373-2384.	7.4	80
6	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. I. Structure and energetics. Journal of Chemical Physics, 2012, 136, 064501.	3.0	58
7	Alkane adsorption in Na-exchanged chabazite: The influence of dispersion forces. Journal of Chemical Physics, 2011, 134, 064102.	3.0	57
8	Cooperative Role of Water Molecules during the Initial Stage of Water-Induced Zeolite Dealumination. ACS Catalysis, 2019, 9, 5119-5135.	11.2	53
9	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. III. Energetics and vibrational spectroscopy of adsorbates. Journal of Chemical Physics, 2012, 136, 064503.	3.0	52
10	Modelling the adsorption of short alkanes in protonated chabazite: The impact of dispersion forces and temperature. Microporous and Mesoporous Materials, 2013, 166, 176-184.	4.4	44
11	Can Dynamics Be Responsible for the Complex Multipeak Infrared Spectra of NO Adsorbed to Copper(II) Sites in Zeolites?. Angewandte Chemie - International Edition, 2015, 54, 7799-7804.	13.8	39
12	Developing a Descriptor-Based Approach for CO and NO Adsorption Strength to Transition Metal Sites in Zeolites. Chemistry of Materials, 2017, 29, 6434-6444.	6.7	34
13	The impact of finite temperature on the coordination of Cu cations in the zeolite SSZ-13. Catalysis Today, 2016, 267, 41-46.	4.4	33
14	Effect of Temperature on the Adsorption of Short Alkanes in the Zeolite SSZ-13â€”Adapting Adsorption Isotherms to Microporous Materials. ACS Catalysis, 2014, 4, 2351-2358.	11.2	32
15	Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13. ACS Catalysis, 2021, 11, 7719-7734.	11.2	31
16	Alignment of semiconducting graphene nanoribbons on vicinal Ge(001). Nanoscale, 2019, 11, 4864-4875.	5.6	26
17	Developing a Thermodynamic Model for the Interactions between Water and Cu in the Zeolite SSZ-13. Journal of Physical Chemistry C, 2017, 121, 6160-6169.	3.1	25
18	Structure and properties of metal-exchanged zeolites studied using gradient-corrected and hybrid functionals. II. Electronic structure and photoluminescence spectra. Journal of Chemical Physics, 2012, 136, 064502.	3.0	24

#	Article	IF	Citations
19	Silicaâ€Grafted Sn^{IV} Catalysts in Hydrogenâ€Transfer Reactions. ChemCatChem, 2015, 7, 3270-3278.	3.7	24
20	Importance of a Nonlocal Description of Electronâ€“Electron Interactions in Modeling the Dissociative Adsorption of H₂ on Cu(100). Journal of Physical Chemistry C, 2014, 118, 5374-5382.	3.1	19
21	UVâ€“Vis and Photoluminescence Spectroscopy to Understand the Coordination of Cu Cations in the Zeolite SSZ-13. Chemistry of Materials, 2019, 31, 9582-9592.	6.7	19
22	Synthesis Gas Conversion over Rh-Mn-W_xC/SiO₂ Catalysts Prepared by Atomic Layer Deposition. ACS Catalysis, 2018, 8, 10707-10720.	11.2	17
23	Anisotropic Synthesis of Armchair Graphene Nanoribbon Arrays from Sub-5 nm Seeds at Variable Pitches on Germanium. Journal of Physical Chemistry Letters, 2019, 10, 4266-4272.	4.6	17
24	Computational description of key spectroscopic features of zeolite SSZ-13. Physical Chemistry Chemical Physics, 2019, 21, 19065-19075.	2.8	11
25	Understanding Waterâ€“Zeolite Interactions: On the Accuracy of Density Functionals. Journal of Physical Chemistry C, 2021, 125, 20261-20274.	3.1	10
26	Diffusion Barriers for Carbon Monoxide on the Cu(001) Surface Using Many-Body Perturbation Theory and Various Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 7862-7872.	5.3	10
27	Verursacht Dynamik das komplexe Infrarotspektrum von NO an Kupfer(II)â€Zentren in Zeolithen?. Angewandte Chemie, 2015, 127, 7910-7915.	2.0	8
28	Exploring driving forces for length growth in graphene nanoribbons during chemical vapor deposition of hydrocarbons on Ge(0Â0Â1) via kinetic Monte Carlo simulations. Applied Surface Science, 2020, 527, 146784.	6.1	8
29	Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2022, 13, 6079-6084.	4.6	8
30	Three Grand Challenges for the Computational Design of Heterogeneous Catalysts. Journal of Physical Chemistry C, 2022, 126, 3305-3313.	3.1	7
31	Identifying hydroxylated copper dimers in SSZ-13 via UV-vis-NIR spectroscopy. Catalysis Science and Technology, 2022, 12, 2744-2748.	4.1	7
32	Silica-Grafted SnIVCatalysts in Hydrogen-Transfer Reactions. ChemCatChem, 2015, 7, 3190-3190.	3.7	0