Carine Michel

List of Publications by Year
in descending order

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101 papers	3,612 citations	117571 34 h-index	149623 56 g-index
118 all docs	118 docs citations	118 times ranked	4553 citing authors

#	Article	IF	Citations
1	Coâ€“Ru Nanoalloy Catalysts for the Acceptorless Dehydrogenation of Alcohols. ACS Applied Nano Materials, 2022, 5, 5733-5744.	2.4	3
2	Mechanistic Investigation and Free Energies of the Reactive Adsorption of Ethanol at the Alumina/Water Interface. Journal of Physical Chemistry C, 2022, 126, 7446-7455.	1.5	8
3	How to Gain Atomistic Insights on Reactions at the Water/Solid Interface?. ACS Catalysis, 2022, 12, 6294-6301.	5.5	17
4	Computational Study of Thermodynamic Overpotentials of Quinone Reduction on Carbon Electrodes to Accelerate Organic Redox Flow Battery Research. ECS Meeting Abstracts, 2022, MA2022-01, 2015-2015.	0.0	0
5	Activity of heterogeneous supported Cu and Ru catalysts in acceptor-less alcohol dehydrogenation. Catalysis Communications, 2021, 148, 106179.	1.6	16
6	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie - International Edition, 2021, 60, 7111-7116.	7.2	7
7	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie, 2021, 133, 7187-7192.	1.6	9
8	The Impact of Water on Ru-Catalyzed Olefin Metathesis: Potent Deactivating Effects Even at Low Water Concentrations. ACS Catalysis, 2021, 11, 893-899.	5.5	25
9	(Dis)Similarities of adsorption of diverse functional groups over alumina and hematite depending on the surface state. Journal of Chemical Physics, 2021, 154, 084701.	1.2	11
10	Influence of Capping Ligands on the Catalytic Performances of Cobalt Nanoparticles Prepared with the Organometallic Route. Journal of Physical Chemistry C, 2021, 125, 7711-7720.	1.5	9
11	RÃ¼cktitelbild: Impact of Organic Templates on the Selective Formation of Zeolite Oligomers (Angew.) Tj ETQq1 1 0.784314 rgBT /O	1.6	0
12	Enantioselective reduction of prochiral ketones promoted by amino amide ruthenium complexes: A DFT study. Journal of Organometallic Chemistry, 2021, 939, 121765.	0.8	1
13	Designing Active Sites for Structure-Sensitive Reactions via the Generalized Coordination Number: Application to Alcohol Dehydrogenation. Journal of Physical Chemistry C, 2021, 125, 10370-10377.	1.5	6
14	DockOnSurf: A Python Code for the High-Throughput Screening of Flexible Molecules Adsorbed on Surfaces. Journal of Chemical Information and Modeling, 2021, 61, 3386-3396.	2.5	13
15	Identification of active catalysts for the acceptorless dehydrogenation of alcohols to carbonyls. Nature Communications, 2021, 12, 5100.	5.8	21
16	Structural Characterization of Phosphate Species Adsorbed on Î³-Alumina by Combining DNP Surface Enhanced NMR Spectroscopy and DFT Calculations. ACS Catalysis, 2021, 11, 11278-11292.	5.5	3
17	Transferable Gaussian Attractive Potentials for Organic/Oxide Interfaces. Journal of Physical Chemistry B, 2021, 125, 10843-10853.	1.2	8
18	Pivotal role of H₂ in the isomerisation of isosorbide over a Ru/C catalyst. Catalysis Science and Technology, 2021, 11, 7973-7981.	2.1	2

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19	Adhesion of lubricant on aluminium through adsorption of additive head-groups on Î³-alumina: A DFT study. Tribology International, 2020, 145, 106140.	3.0	15
20	Solvation Free Energies and Adsorption Energies at the Metal/Water Interface from Hybrid Quantum-Mechanical/Molecular Mechanics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6539-6549.	2.3	34
21	Demystifying the Atomistic Origin of the Electric Field Effect on Methane Oxidation. Journal of Physical Chemistry Letters, 2020, 11, 6976-6981.	2.1	16
22	Strong Affinity of Triazolium-Appended Dipyrromethenes (TADs) for BF4â^'. Molecules, 2020, 25, 4555.	1.7	2
23	Ten Facets, One Force Field: The GAL19 Force Field for Waterâ€“Noble Metal Interfaces. Journal of Chemical Theory and Computation, 2020, 16, 4565-4578.	2.3	26
24	Elucidating the role of electrochemical polarization on the selectivity of the CO2 hydrogenation reaction over Ru. Electrochimica Acta, 2020, 350, 136405.	2.6	20
25	Hydroxide-Induced Degradation of Olefin Metathesis Catalysts: A Challenge for Metathesis in Alkaline Media. ACS Catalysis, 2020, 10, 3838-3843.	5.5	15
26	Supported Cobalt Catalysts for Acceptorless Alcohol Dehydrogenation. ChemPlusChem, 2020, 85, 1315-1324.	1.3	16
27	Acidic Properties of Alkaline-Earth Phosphates Determined by an Experimental-Theoretical Approach. Journal of Physical Chemistry C, 2020, 124, 2013-2023.	1.5	3
28	Two-sites are better than one: revisiting the OER mechanism on CoOOH by DFT with electrode polarization. Physical Chemistry Chemical Physics, 2020, 22, 7031-7038.	1.3	45
29	Importance of the decoration in shaped cobalt nanoparticles in the acceptor-less secondary alcohol dehydrogenation. Catalysis Science and Technology, 2020, 10, 4923-4937.	2.1	14
30	Understanding the influence of the composition of the Ag Pd catalysts on the selective formic acid decomposition and subsequent levulinic acid hydrogenation. International Journal of Hydrogen Energy, 2020, 45, 17339-17353.	3.8	29
31	Production of 1,3-butadiene in one step catalytic dehydration of 2,3-butanediol. Catalysis Today, 2019, 323, 62-68.	2.2	26
32	Rational design of selective metal catalysts for alcohol amination with ammonia. Nature Catalysis, 2019, 2, 773-779.	16.1	70
33	Reactivity of shape-controlled crystals and metadynamics simulations locate the weak spots of alumina in water. Nature Communications, 2019, 10, 3139.	5.8	42
34	AuCu/CeO2 bimetallic catalysts for the selective oxidation of fatty alcohol ethoxylates to alkyl ether carboxylic acids. Journal of Catalysis, 2019, 380, 132-144.	3.1	6
35	Evaluating Thermal Corrections for Adsorption Processes at the Metal/Gas Interface. Journal of Physical Chemistry C, 2019, 123, 28828-28835.	1.5	17
36	New process for producing butane-2,3-dione by oxidative dehydrogenation of 3-hydroxybutanone. Reaction Chemistry and Engineering, 2019, 4, 932-938.	1.9	3

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37	Theoretical insight into the origin of the electrochemical promotion of ethylene oxidation on ruthenium oxide. Catalysis Science and Technology, 2019, 9, 5915-5926.	2.1	26
38	Can microsolvation effects be estimated from vacuum computations? A case-study of alcohol decomposition at the H₂O/Pt(111) interface. Physical Chemistry Chemical Physics, 2019, 21, 5368-5377.	1.3	25
39	C6 Diacids from homocitric acid lactone using relay heterogeneous catalysis in water. Catalysis Today, 2019, 319, 191-196.	2.2	1
40	Computational screening for selective catalysts: Cleaving the C C bond during ethanol electro-oxidation reaction. Electrochimica Acta, 2018, 274, 274-278.	2.6	26
41	Rational design of heterogeneous catalysts for biomass conversion â€“ Inputs from computational chemistry. Current Opinion in Green and Sustainable Chemistry, 2018, 10, 51-59.	3.2	17
42	Unsupported shaped cobalt nanoparticles as efficient and recyclable catalysts for the solvent-free acceptorless dehydrogenation of alcohols. Catalysis Science and Technology, 2018, 8, 562-572.	2.1	20
43	Force Field for Water over Pt(111): Development, Assessment, and Comparison. Journal of Chemical Theory and Computation, 2018, 14, 3238-3251.	2.3	38
44	Structuration and Dynamics of Interfacial Liquid Water at Hydrated Î³-Alumina Determined by ab Initio Molecular Simulations: Implications for Nanoparticle Stability. ACS Applied Nano Materials, 2018, 1, 191-199.	2.4	37
45	Direct n-octanol amination by ammonia on supported Ni and Pd catalysts: activity is enhanced by â€œspectatorâ€•ammonia adsorbates. Catalysis Science and Technology, 2018, 8, 611-621.	2.1	26
46	Trends and Control in the Nitridation of Transition-Metal Surfaces. ACS Catalysis, 2018, 8, 63-68.	5.5	19
47	Unraveling the Role of Base and Catalyst Polarization in Alcohol Oxidation on Au and Pt in Water. ACS Catalysis, 2018, 8, 11716-11721.	5.5	31
48	DFT investigations for the catalytic reaction mechanism of methane combustion occurring on Pd(<scp>ii</scp>)/Al-MCM-41. Physical Chemistry Chemical Physics, 2018, 20, 25377-25386.	1.3	8
49	Adsorption and Decomposition of Formic Acid on Cobalt(0001). Journal of Physical Chemistry C, 2018, 122, 20279-20288.	1.5	16
50	Câ€“H Activation and Proton Transfer Initiate Alkene Metathesis Activity of the Tungsten(IV)â€“Oxo Complex. Journal of the American Chemical Society, 2018, 140, 11395-11401.	6.6	21
51	Direct Amination of Alcohols Catalyzed by Aluminum Triflate: Anâ€‰Experimental and Computational Study. Chemistry - A European Journal, 2018, 24, 14146-14153.	1.7	13
52	Supported goldâ€“nickel nano-alloy as a highly efficient catalyst in levulinic acid hydrogenation with formic acid as an internal hydrogen source. Catalysis Science and Technology, 2018, 8, 4318-4331.	2.1	51
53	Key Role of Anionic Doping for H₂ Production from Formic Acid on Pd(111). ACS Catalysis, 2017, 7, 1955-1959.	5.5	72
54	CO Chemisorption on Ultrathin MgO-Supported Palladium Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 5551-5564.	1.5	17

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55	Adsorption and Decomposition of a Lignin Î²-O-4 Linkage Model, 2-Phenoxyethanol, on Pt(111): Combination of Experiments and First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 9889-9900.	1.5	16
56	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). Journal of Physical Chemistry C, 2017, 121, 21510-21519.	1.5	27
57	Molecular mechanics models for the image charge, a comment on â€œincluding image charge effects in the molecular dynamics simulations of molecules on metal surfacesâ€. Journal of Computational Chemistry, 2017, 38, 2127-2129.	1.5	9
58	Controlling the Adsorption of Aromatic Compounds on Pt(111) with Oxygenate Substituents: From DFT to Simple Molecular Descriptors. Journal of Physical Chemistry Letters, 2016, 7, 2074-2079.	2.1	23
59	Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites. ACS Catalysis, 2016, 6, 8404-8409.	5.5	83
60	Decomposition Mechanism of Anisole on Pt(111): Combining Single-Crystal Experiments and First-Principles Calculations. ACS Catalysis, 2016, 6, 8166-8178.	5.5	34
61	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. Physical Chemistry Chemical Physics, 2016, 18, 31850-31861.	1.3	80
62	Towards more accurate prediction of activation energies for polyalcohol dehydrogenation on transition metal catalysts in water. Catalysis Science and Technology, 2016, 6, 6615-6624.	2.1	31
63	Ethanol Electro-oxidation on Palladium Revisited Using Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS) and Density Functional Theory (DFT): Why Is It Difficult To Break the Câ€“C Bond?. ACS Catalysis, 2016, 6, 4894-4906.	5.5	109
64	Study of a novel hepta-coordinated FeIII bimetallic complex with an unusual 1,2,4,5-tetrazine-ring opening. Polyhedron, 2016, 108, 163-168.	1.0	13
65	Electro-carboxylation of butadiene and ethene over Pt and Ni catalysts. Journal of Catalysis, 2016, 343, 240-247.	3.1	31
66	Ru catalysts for levulinic acid hydrogenation with formic acid as a hydrogen source. Green Chemistry, 2016, 18, 2014-2028.	4.6	126
67	Modeling the HCOOH/CO₂ Electrocatalytic Reaction: When Details Are Key. ChemPhysChem, 2015, 16, 2307-2311.	1.0	44
68	In Silico Screening of Iron-Oxo Catalysts for CH Bond Cleavage. ACS Catalysis, 2015, 5, 2490-2499.	5.5	35
69	Why Is Ruthenium an Efficient Catalyst for the Aqueous-Phase Hydrogenation of Biosourced Carbonyl Compounds?. ACS Catalysis, 2015, 5, 4130-4132.	5.5	158
70	Trade-Off between Accuracy and Universality in Linear Energy Relations for Alcohol Dehydrogenation on Transition Metals. Journal of Physical Chemistry C, 2015, 119, 12988-12998.	1.5	46
71	Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 13949-13963.	1.3	90
72	Molecular adsorption at Pt(111). How accurate are DFT functionals?. Physical Chemistry Chemical Physics, 2015, 17, 28921-28930.	1.3	210

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73	Proton Transfer in Aqueous Solution: Exploring the Boundaries of Adaptive QM/MM. Challenges and Advances in Computational Chemistry and Physics, 2015, , 51-91.	0.6	17
74	Formation of Acrylates from Ethylene and CO₂ on Ni Complexes: A Mechanistic Viewpoint from a Hybrid DFT Approach. Organometallics, 2014, 33, 6369-6380.	1.1	36
75	Control of the anisotropic shape of cobalt nanorods in the liquid phase: from experiment to theoryâ€¦ and back. Nanoscale, 2014, 6, 2682.	2.8	39
76	Linear Energy Relations As Predictive Tools for Polyalcohol Catalytic Reactivity. ACS Catalysis, 2014, 4, 464-468.	5.5	41
77	Role of water in metal catalyst performance for ketone hydrogenation: a joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone. Chemical Communications, 2014, 50, 12450-12453.	2.2	168
78	Multiscale Modeling of Chemistry in Water: Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 5567-5577.	2.3	59
79	Tuning catalytic reactivity on metal surfaces: Insights from DFT. Journal of Catalysis, 2013, 308, 374-385.	3.1	29
80	On the key role of hydroxyl groups in platinum-catalysed alcohol oxidation in aqueous medium. Catalysis Science and Technology, 2013, 3, 339-350.	2.1	51
81	Early stages of water/hydroxyl phase generation at transition metal surfaces â€“ synergetic adsorption and Oâ€“H bond dissociation assistance. Physical Chemistry Chemical Physics, 2012, 14, 15286.	1.3	28
82	Energy extrapolation schemes for adaptive multi-scale molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 074111.	1.2	12
83	Heterogeneous Transformation of Glycerol to Lactic Acid. Topics in Catalysis, 2012, 55, 474-479.	1.3	60
84	Câ€“H versus Oâ€“H Bond Dissociation for Alcohols on a Rh(111) Surface: A Strong Assistance from Hydrogen Bonded Neighbors. ACS Catalysis, 2011, 1, 1430-1440.	5.5	85
85	Cu(bipy)²⁺/TEMPO-Catalyzed Oxidation of Alcohols: Radical or Nonradical Mechanism?. Inorganic Chemistry, 2011, 50, 11896-11904.	1.9	43
86	Unraveling Gold(I)â€Specific Action Towards Peptidic Disulfide Cleavage: A DFT Investigation. ChemPhysChem, 2011, 12, 2596-2603.	1.0	2
87	Unravelling the Mechanism of Glycerol Hydrogenolysis over Rhodium Catalyst through Combined Experimentalâ€“Theoretical Investigations. Chemistry - A European Journal, 2011, 17, 14288-14299.	1.7	99
88	Biasâ€exchange metadynamics applied to the study of chemical reactivity. International Journal of Quantum Chemistry, 2010, 110, 2299-2307.	1.0	2
89	A high performance grid-based algorithm for computing QTAIM properties. Chemical Physics Letters, 2009, 472, 149-152.	1.2	151
90	What Singles out the FeO²⁺Moiety? A Density-Functional Theory Study of the Methane-to-Methanol Reaction Catalyzed by the First Row Transition-Metal Oxide Dications MO(H₂O)_p²⁺, M = Vâ€¦Cu. Inorganic Chemistry, 2009, 48, 3628-3638.	1.9	71

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91	Tracing the Entropy along a Reactive Pathway: The Energy As a Generalized Reaction Coordinate. Journal of Chemical Theory and Computation, 2009, 5, 2193-2196.	2.3	15
92	Activation of the Câ^'H Bond by Electrophilic Attack: Theoretical Study of the Reaction Mechanism of the Aerobic Oxidation of Alcohols to Aldehydes by the Cu(bipy)²⁺/2,2,6,6-Tetramethylpiperidinyl-1-oxy Cocatalyst System. Inorganic Chemistry, 2009, 48, 11909-11920.	1.9	89
93	A DFT study of 1,3-dipolar cycloaddition reactions of 5-membered cyclic nitrones with Î±,Î²-unsaturated lactones and with cyclic vinyl ethers: Part 1. Tetrahedron: Asymmetry, 2008, 19, 1660-1669.	1.8	16
94	A DFT study of 1,3-dipolar cycloadditions of cyclic nitrones to unsaturated lactones. Part II. Tetrahedron: Asymmetry, 2008, 19, 2140-2148.	1.8	19
95	Free energy calculation of the effects of the fluorinated phosphorus ligands on the Câ€“H and Câ€“C reductive elimination from Pt(IV). Computational and Theoretical Chemistry, 2008, 852, 54-61.	1.5	8
96	Synthesis of N-acridinyl-Nâ€²-alkylguanidines: Dramatic influence of amine to guanidine replacement on the physicochemical properties. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4779-4782.	1.0	4
97	Free Energyab InitioMetadynamics:Â A New Tool for the Theoretical Study of Organometallic Reactivity? Example of the Câ^'C and Câ^'H Reductive Eliminations from Platinum(IV) Complexes. Organometallics, 2007, 26, 1241-1249.	1.1	37
98	Structural, Kinetic, and Theoretical Studies on Models of the Zincâ€Containing Phosphodiesterase Active Center: Mediumâ€Dependent Reaction Mechanisms. Chemistry - A European Journal, 2007, 13, 9093-9106.	1.7	49
99	Silver versus Gold Catalysis in Tandem Reactions of Carbonyl Functions onto Alkynes: A Versatile Access to Furoquinoline and Pyranoquinoline Cores. Chemistry - A European Journal, 2007, 13, 5632-5641.	1.7	155
100	Theoretical study of the cyclization of carbonyl groups on unactivated alkynyl-quinolines in the gas phase and in methanol solution. Computational and Theoretical Chemistry, 2007, 811, 175-182.	1.5	5
101	First Câ€“C bond formation in the Pausonâ€“Khand reaction: Influence of carbonâ€“carbon triple bond polarization on regiochemistry. Journal of Organometallic Chemistry, 2006, 691, 4281-4288.	0.8	35