

# Stephan N Steinmann

## List of Publications by Year in descending order

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93  
papers

5,345  
citations

117571

34  
h-index

85498

71  
g-index

109  
all docs

109  
docs citations

109  
times ranked

6934  
citing authors

#	ARTICLE	IF	CITATIONS
1	How are transition states modeled in heterogeneous electrocatalysis?. <i>Current Opinion in Electrochemistry</i> , 2022, 33, 100940.	2.5	20
2	Autonomous high-throughput computations in catalysis. <i>Chem Catalysis</i> , 2022, 2, 940-956.	2.9	14
3	Genesis of MoS <sub>2</sub> from model-Mo-oxide precursors supported on $\gamma$ -alumina. <i>Journal of Catalysis</i> , 2022, 408, 303-315.	3.1	4
4	Mechanistic Investigation and Free Energies of the Reactive Adsorption of Ethanol at the Alumina/Water Interface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 7446-7455.	1.5	8
5	How to Gain Atomistic Insights on Reactions at the Water/Solid Interface?. <i>ACS Catalysis</i> , 2022, 12, 6294-6301.	5.5	17
6	Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6079-6084.	2.1	8
7	Atomistic modeling of electrocatalysis: Are we there yet?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1499.	6.2	79
8	The Impact of Water on Ru-Catalyzed Olefin Metathesis: Potent Deactivating Effects Even at Low Water Concentrations. <i>ACS Catalysis</i> , 2021, 11, 893-899.	5.5	25
9	Nature of High- and Low-Affinity Metal Surface Sites on Birnessite Nanosheets. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 66-76.	1.2	11
10	(Dis)Similarities of adsorption of diverse functional groups over alumina and hematite depending on the surface state. <i>Journal of Chemical Physics</i> , 2021, 154, 084701.	1.2	11
11	Understanding electrified interfaces. <i>Nature Reviews Materials</i> , 2021, 6, 289-291.	23.3	38
12	Designing Active Sites for Structure-Sensitive Reactions via the Generalized Coordination Number: Application to Alcohol Dehydrogenation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10370-10377.	1.5	6
13	Efficient recursive least squares solver for rank-deficient matrices. <i>Applied Mathematics and Computation</i> , 2021, 399, 125996.	1.4	0
14	DockOnSurf: A Python Code for the High-Throughput Screening of Flexible Molecules Adsorbed on Surfaces. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3386-3396.	2.5	13
15	How Stable Are 2H-MoS <sub>2</sub> Edges under Hydrogen Evolution Reaction Conditions?. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17058-17067.	1.5	25
16	Transferable Gaussian Attractive Potentials for Organic/Oxide Interfaces. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10843-10853.	1.2	8
17	What does graphitic carbon nitride really look like?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2853-2859.	1.3	12
18	Same ligand, three first-row metals: comparing M-amido bifunctional reactivity (Mn, Fe, Co). <i>Dalton Transactions</i> , 2021, 50, 14542-14546.	1.6	5

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19	Adhesion of lubricant on aluminium through adsorption of additive head-groups on $\gamma$ -alumina: A DFT study. <i>Tribology International</i> , 2020, 145, 106140.	3.0	15
20	Mononuclear Fe in N-doped carbon: computational elucidation of active sites for electrochemical oxygen reduction and oxygen evolution reactions. <i>Catalysis Science and Technology</i> , 2020, 10, 1006-1014.	2.1	34
21	Solvation Free Energies and Adsorption Energies at the Metal/Water Interface from Hybrid Quantum-Mechanical/Molecular Mechanics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6539-6549.	2.3	34
22	Water adlayers on noble metal surfaces: Insights from energy decomposition analysis. <i>Journal of Chemical Physics</i> , 2020, 153, 054703.	1.2	10
23	Demystifying the Atomistic Origin of the Electric Field Effect on Methane Oxidation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6976-6981.	2.1	16
24	Size-Dependent Structural, Energetic, and Spectroscopic Properties of $\text{MoS}_3$ Polymorphs. <i>Crystal Growth and Design</i> , 2020, 20, 7750-7760.	1.4	9
25	Strong Affinity of Triazolium-Appended Dipyrromethenes (TADs) for $\text{BF}_4^-$ . <i>Molecules</i> , 2020, 25, 4555.	1.7	2
26	Ten Facets, One Force Field: The GAL19 Force Field for Water@Noble Metal Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4565-4578.	2.3	26
27	Elucidating the role of electrochemical polarization on the selectivity of the $\text{CO}_2$ hydrogenation reaction over Ru. <i>Electrochimica Acta</i> , 2020, 350, 136405.	2.6	20
28	Revisiting the Active Sites at the $\text{MoS}_2/\text{H}_2\text{O}$ Interface via Grand-Canonical DFT: The Role of Water Dissociation. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 31401-31410.	4.0	36
29	Hydroxide-Induced Degradation of Olefin Metathesis Catalysts: A Challenge for Metathesis in Alkaline Media. <i>ACS Catalysis</i> , 2020, 10, 3838-3843.	5.5	15
30	Two-sites are better than one: revisiting the OER mechanism on $\text{CoOOH}$ by DFT with electrode polarization. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7031-7038.	1.3	45
31	The Mode of Incorporation of As(-I) and Se(-I) in Natural Pyrite Revisited. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 379-390.	1.2	18
32	Parameter-free coordination numbers for solutions and interfaces. <i>Journal of Chemical Physics</i> , 2020, 152, 024124.	1.2	11
33	Revisiting the Atomistic Structures at the Interface of Au(111) Electrode@Sulfuric Acid Solution. <i>Journal of the American Chemical Society</i> , 2020, 142, 9439-9446.	6.6	35
34	Evaluating Thermal Corrections for Adsorption Processes at the Metal/Gas Interface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28828-28835.	1.5	17
35	The Pressure Gap for Thiols: Methanethiol Self-Assembly on Au(111) from Vacuum to 1 bar. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12382-12389.	1.5	7
36	Theory and experiments join forces to characterize the electrocatalytic interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 7611-7613.	3.3	5

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37	Theory-guided materials design: two-dimensional MXenes in electro- and photocatalysis. <i>Nanoscale Horizons</i> , 2019, 4, 809-827.	4.1	218
38	Theoretical insight into the origin of the electrochemical promotion of ethylene oxidation on ruthenium oxide. <i>Catalysis Science and Technology</i> , 2019, 9, 5915-5926.	2.1	26
39	Implicit self-consistent electrolyte model in plane-wave density-functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 234101.	1.2	561
40	Energy Decomposition Analysis for Metal Surface-Adsorbate Interactions by Block Localized Wave Functions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 265-275.	2.3	13
41	Can microsolvation effects be estimated from vacuum computations? A case-study of alcohol decomposition at the $H_2O/Pt(111)$ interface. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5368-5377.	1.3	25
42	C6 Diacids from homocitric acid lactone using relay heterogeneous catalysis in water. <i>Catalysis Today</i> , 2019, 319, 191-196.	2.2	1
43	Computational screening for selective catalysts: Cleaving the C-C bond during ethanol electro-oxidation reaction. <i>Electrochimica Acta</i> , 2018, 274, 274-278.	2.6	26
44	Evaluating the Risk of C-C Bond Formation during Selective Hydrogenation of Acetylene on Palladium. <i>ACS Catalysis</i> , 2018, 8, 1662-1671.	5.5	65
45	Force Field for Water over Pt(111): Development, Assessment, and Comparison. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3238-3251.	2.3	38
46	Tetrazine-Based Ligand Transformation Driving Metal-Metal Bond and Mixed-Valence $Hg^{I}/Hg^{II}$ . <i>ACS Omega</i> , 2018, 3, 10273-10277.	1.6	3
47	Shining Light on Carbon Nitrides: Leveraging Temperature To Understand Optical Gap Variations. <i>Chemistry of Materials</i> , 2018, 30, 4253-4262.	3.2	28
48	Acetylene Adsorption on Pd-Ag Alloys: Evidence for Limited Island Formation and Strong Reverse Segregation from Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15456-15463.	1.5	35
49	Key Role of Anionic Doping for $H_2$ Production from Formic Acid on Pd(111). <i>ACS Catalysis</i> , 2017, 7, 1955-1959.	5.5	72
50	Challenges in calculating the bandgap of triazine-based carbon nitride structures. <i>Journal of Materials Chemistry A</i> , 2017, 5, 5115-5122.	5.2	34
51	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). <i>Journal of Physical Chemistry C</i> , 2017, 121, 21510-21519.	1.5	27
52	Molecular mechanics models for the image charge, a comment on including image charge effects in the molecular dynamics simulations of molecules on metal surfaces. <i>Journal of Computational Chemistry</i> , 2017, 38, 2127-2129.	1.5	9
53	A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers. <i>Journal of Chemical Physics</i> , 2017, 147, 054106.	1.2	31
54	DFT Perspective on the Thermochemistry of Carbon Nitride Synthesis. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24542-24550.	1.5	21

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55	C <sub>2</sub> H <sub>2</sub> -Induced Surface Restructuring of Pd-Ag Catalysts: Insights from Theoretical Modeling. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26320-26327.	1.5	26
56	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31850-31861.	1.3	80
57	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 C-C Bond?. <i>ACS Catalysis</i> , 2016, 6, 4894-4906.	5.5	109
58	Study of a novel hepta-coordinated FeIII bimetallic complex with an unusual 1,2,4,5-tetrazine-ring opening. <i>Polyhedron</i> , 2016, 108, 163-168.	1.0	13
59	Electro-carboxylation of butadiene and ethene over Pt and Ni catalysts. <i>Journal of Catalysis</i> , 2016, 343, 240-247.	3.1	31
60	Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5619-5623.	1.5	78
61	A fast charge-Dependent atom-pairwise dispersion correction for DFTB3. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1265-1272.	1.0	16
62	Modeling the HCOOH/CO <sub>2</sub> Electrocatalytic Reaction: When Details Are Key. <i>ChemPhysChem</i> , 2015, 16, 2307-2311.	1.0	44
63	Impacts of electrode potentials and solvents on the electroreduction of CO <sub>2</sub> : a comparison of theoretical approaches. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13949-13963.	1.3	90
64	Relationship between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25188-25196.	1.5	104
65	Molecular adsorption at Pt(111). How accurate are DFT functionals?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28921-28930.	1.3	210
66	How important is self-consistency for the dDsC density dependent dispersion correction?. <i>Journal of Chemical Physics</i> , 2014, 140, 18A516.	1.2	24
67	Layer-Dependent Electrocatalysis of MoS <sub>2</sub> for Hydrogen Evolution. <i>Nano Letters</i> , 2014, 14, 553-558.	4.5	667
68	Hierarchically Structured Microfibers of "Single Stack" Perylene Bisimide and Quaterthiophene Nanowires. <i>ACS Nano</i> , 2013, 7, 8498-8508.	7.3	88
69	Bonding analysis of planar hypercoordinate atoms via the generalized BLW-LOL. <i>Journal of Computational Chemistry</i> , 2013, 34, 2242-2248.	1.5	10
70	Wave function methods for fractional electrons. <i>Journal of Chemical Physics</i> , 2013, 139, 074107.	1.2	19
71	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. <i>Journal of Chemical Physics</i> , 2013, 139, 104112.	1.2	51
72	Dynamical second-order Bethe-Salpeter equation kernel: A method for electronic excitation beyond the adiabatic approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 154109.	1.2	23

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73	Benchmark tests and spin adaptation for the particle-particle random phase approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 174110.	1.2	40
74	A ratiometric fluorescence sensor for caffeine. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7487.	1.5	19
75	Role of $\pi$ -Acceptor Effects in Controlling the Lability of Novel Monofunctional Pt(II) and Pd(II) Complexes: Crystal Structure of [Pt(triipyridinedimethane)Cl]Cl. <i>Inorganic Chemistry</i> , 2012, 51, 1516-1529.	1.9	48
76	$\pi$ -Depletion as a criterion to predict $\pi$ -stacking ability. <i>Chemical Communications</i> , 2012, 48, 9239.	2.2	68
77	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4305-4316.	2.3	38
78	Quantification of "fuzzy" chemical concepts: a computational perspective. <i>Chemical Society Reviews</i> , 2012, 41, 4671.	18.7	108
79	How are small endohedral silicon clusters stabilized?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14842.	1.3	12
80	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1629-1640.	2.3	153
81	Fluorescence sensing of caffeine in water with polysulfonated pyrenes. <i>Chemical Communications</i> , 2011, 47, 10584.	2.2	43
82	Dispersion-Corrected Energy Decomposition Analysis for Intermolecular Interactions Based on the BLW and dDXDM Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5467-5477.	1.1	43
83	The norbornene mystery revealed. <i>Chemical Communications</i> , 2011, 47, 227-229.	2.2	20
84	How do electron localization functions describe $\pi$ -electron delocalization?. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20584.	1.3	99
85	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3567-3577.	2.3	400
86	A Density Dependent Dispersion Correction. <i>Chimia</i> , 2011, 65, 240.	0.3	40
87	A generalized-gradient approximation exchange hole model for dispersion coefficients. <i>Journal of Chemical Physics</i> , 2011, 134, 044117.	1.2	270
88	Overcoming systematic DFT errors for hydrocarbon reaction energies. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 429-442.	0.5	51
89	Branched Alkanes Have Contrasting Stabilities. <i>Organic Letters</i> , 2010, 12, 3070-3073.	2.4	34
90	How Strained are Carbomeric-Cycloalkanes?. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6705-6712.	1.1	22

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91	A System-Dependent Density-Based Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1990-2001.	2.3	133
92	Direct Assessment of Electron Delocalization Using NMR Chemical Shifts. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9828-9833.	7.2	49
93	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2950-2958.	2.3	76