Stephan N Steinmann

List of Publications by Year
in descending order

		117625	85541
93 papers	5,345 citations	34 h-index	71 g-index

109 all docs	109 docs citations	109 times ranked	6934 citing authors

#	Article	IF	Citations
1	Layer-Dependent Electrocatalysis of MoS₂ for Hydrogen Evolution. Nano Letters, 2014, 14, 553-558.	9.1	667
2	Implicit self-consistent electrolyte model in plane-wave density-functional theory. Journal of Chemical Physics, 2019, 151, 234101.	3.0	561
3	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. Journal of Chemical Theory and Computation, 2011, 7, 3567-3577.	5.3	400
4	A generalized-gradient approximation exchange hole model for dispersion coefficients. Journal of Chemical Physics, 2011, 134, 044117.	3.0	270
5	Theory-guided materials design: two-dimensional MXenes in electro- and photocatalysis. Nanoscale Horizons, 2019, 4, 809-827.	8.0	218
6	Molecular adsorption at Pt(111). How accurate are DFT functionals?. Physical Chemistry Chemical Physics, 2015, 17, 28921-28930.	2.8	210
7	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. Journal of Chemical Theory and Computation, 2012, 8, 1629-1640.	5.3	153
8	A System-Dependent Density-Based Dispersion Correction. Journal of Chemical Theory and Computation, 2010, 6, 1990-2001.	5.3	133
9	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.	11.2	109
10	Quantification of â€œfuzzyâ€•chemical concepts: a computational perspective. Chemical Society Reviews, 2012, 41, 4671.	38.1	108
11	Relationship between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective. Journal of Physical Chemistry C, 2015, 119, 25188-25196.	3.1	104
12	How do electron localization functions describe Ï€-electron delocalization?. Physical Chemistry Chemical Physics, 2011, 13, 20584.	2.8	99
13	Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 13949-13963.	2.8	90
14	Hierarchically Structured Microfibers of â€œSingle Stackâ€•Perylene Bisimide and Quaterthiophene Nanowires. ACS Nano, 2013, 7, 8498-8508.	14.6	88
15	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. Physical Chemistry Chemical Physics, 2016, 18, 31850-31861.	2.8	80
16	Atomistic modeling of electrocatalysis: Are we there yet?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1499.	14.6	79
17	Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. Journal of Physical Chemistry C, 2016, 120, 5619-5623.	3.1	78
18	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2950-2958.	5.3	76

#	ARTICLE	IF	CITATIONS
19	Key Role of Anionic Doping for H₂ Production from Formic Acid on Pd(111). ACS Catalysis, 2017, 7, 1955-1959.	11.2	72
20	Ï€-Depletion as a criterion to predict Ï€-stacking ability. Chemical Communications, 2012, 48, 9239.	4.1	68
21	Evaluating the Risk of Câ€“C Bond Formation during Selective Hydrogenation of Acetylene on Palladium. ACS Catalysis, 2018, 8, 1662-1671.	11.2	65
22	Overcoming systematic DFT errors for hydrocarbon reaction energies. Theoretical Chemistry Accounts, 2010, 127, 429-442.	1.4	51
23	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. Journal of Chemical Physics, 2013, 139, 104112.	3.0	51
24	Direct Assessment of Electron Delocalization Using NMR Chemical Shifts. Angewandte Chemie - International Edition, 2009, 48, 9828-9833.	13.8	49
25	Role of Ï€-Acceptor Effects in Controlling the Lability of Novel Monofunctional Pt(II) and Pd(II) Complexes: Crystal Structure of [Pt(tripyridinedimethane)Cl]Cl. Inorganic Chemistry, 2012, 51, 1516-1529.	4.0	48
26	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.	2.8	45
27	Modeling the HCOOH/CO₂ Electrocatalytic Reaction: When Details Are Key. ChemPhysChem, 2015, 16, 2307-2311.	2.1	44
28	Fluorescence sensing of caffeine in water with polysulfonated pyrenes. Chemical Communications, 2011, 47, 10584.	4.1	43
29	Dispersion-Corrected Energy Decomposition Analysis for Intermolecular Interactions Based on the BLW and dDXDM Methods. Journal of Physical Chemistry A, 2011, 115, 5467-5477.	2.5	43
30	A Density Dependent Dispersion Correction. Chimia, 2011, 65, 240.	0.6	40
31	Benchmark tests and spin adaptation for the particle-particle random phase approximation. Journal of Chemical Physics, 2013, 139, 174110.	3.0	40
32	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. Journal of Chemical Theory and Computation, 2012, 8, 4305-4316.	5.3	38
33	Force Field for Water over Pt(111): Development, Assessment, and Comparison. Journal of Chemical Theory and Computation, 2018, 14, 3238-3251.	5.3	38
34	Understanding electrified interfaces. Nature Reviews Materials, 2021, 6, 289-291.	48.7	38
35	Revisiting the Active Sites at the MoS₂/H₂O Interface via Grand-Canonical DFT: The Role of Water Dissociation. ACS Applied Materials & Interfaces, 2020, 12, 31401-31410.	8.0	36
36	Acetylene Adsorption on Pdâ€“Ag Alloys: Evidence for Limited Island Formation and Strong Reverse Segregation from Monte Carlo Simulations. Journal of Physical Chemistry C, 2018, 122, 15456-15463.	3.1	35

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37	Revisiting the Atomistic Structures at the Interface of Au(111) Electrodeâ€“Sulfuric Acid Solution. Journal of the American Chemical Society, 2020, 142, 9439-9446.	13.7	35
38	Branched Alkanes Have Contrasting Stabilities. Organic Letters, 2010, 12, 3070-3073.	4.6	34
39	Challenges in calculating the bandgap of triazine-based carbon nitride structures. Journal of Materials Chemistry A, 2017, 5, 5115-5122.	10.3	34
40	Mononuclear Fe in N-doped carbon: computational elucidation of active sites for electrochemical oxygen reduction and oxygen evolution reactions. Catalysis Science and Technology, 2020, 10, 1006-1014.	4.1	34
41	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.	5.3	34
42	Electro-carboxylation of butadiene and ethene over Pt and Ni catalysts. Journal of Catalysis, 2016, 343, 240-247.	6.2	31
43	A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers. Journal of Chemical Physics, 2017, 147, 054106.	3.0	31
44	Shining Light on Carbon Nitrides: Leveraging Temperature To Understand Optical Gap Variations. Chemistry of Materials, 2018, 30, 4253-4262.	6.7	28
45	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). Journal of Physical Chemistry C, 2017, 121, 21510-21519.	3.1	27
46	C₂H₂-Induced Surface Restructuring of Pdâ€“Ag Catalysts: Insights from Theoretical Modeling. Journal of Physical Chemistry C, 2016, 120, 26320-26327.	3.1	26
47	Computational screening for selective catalysts: Cleaving the C C bond during ethanol electro-oxidation reaction. Electrochimica Acta, 2018, 274, 274-278.	5.2	26
48	Theoretical insight into the origin of the electrochemical promotion of ethylene oxidation on ruthenium oxide. Catalysis Science and Technology, 2019, 9, 5915-5926.	4.1	26
49	Ten Facets, One Force Field: The GAL19 Force Field for Waterâ€“Noble Metal Interfaces. Journal of Chemical Theory and Computation, 2020, 16, 4565-4578.	5.3	26
50	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.	2.8	25
51	The Impact of Water on Ru-Catalyzed Olefin Metathesis: Potent Deactivating Effects Even at Low Water Concentrations. ACS Catalysis, 2021, 11, 893-899.	11.2	25
52	How Stable Are 2H-MoS₂ Edges under Hydrogen Evolution Reaction Conditions?. Journal of Physical Chemistry C, 2021, 125, 17058-17067.	3.1	25
53	How important is self-consistency for the dDsC density dependent dispersion correction?. Journal of Chemical Physics, 2014, 140, 18A516.	3.0	24
54	Dynamical second-order Bethe-Salpeter equation kernel: A method for electronic excitation beyond the adiabatic approximation. Journal of Chemical Physics, 2013, 139, 154109.	3.0	23

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55	How Strained are Carbomeric-Cycloalkanes?. Journal of Physical Chemistry A, 2010, 114, 6705-6712.	2.5	22
56	DFT Perspective on the Thermochemistry of Carbon Nitride Synthesis. Journal of Physical Chemistry C, 2016, 120, 24542-24550.	3.1	21
57	The norbornene mystery revealed. Chemical Communications, 2011, 47, 227-229.	4.1	20
58	Elucidating the role of electrochemical polarization on the selectivity of the CO2 hydrogenation reaction over Ru. Electrochimica Acta, 2020, 350, 136405.	5.2	20
59	How are transition states modeled in heterogeneous electrocatalysis?. Current Opinion in Electrochemistry, 2022, 33, 100940.	4.8	20
60	A ratiometric fluorescence sensor for caffeine. Organic and Biomolecular Chemistry, 2012, 10, 7487.	2.8	19
61	Wave function methods for fractional electrons. Journal of Chemical Physics, 2013, 139, 074107.	3.0	19
62	The Mode of Incorporation of As(-I) and Se(-I) in Natural Pyrite Revisited. ACS Earth and Space Chemistry, 2020, 4, 379-390.	2.7	18
63	Evaluating Thermal Corrections for Adsorption Processes at the Metal/Gas Interface. Journal of Physical Chemistry C, 2019, 123, 28828-28835.	3.1	17
64	How to Gain Atomistic Insights on Reactions at the Water/Solid Interface?. ACS Catalysis, 2022, 12, 6294-6301.	11.2	17
65	A fast chargeâ€Dependent atomâ€pairwise dispersion correction for DFTB3. International Journal of Quantum Chemistry, 2015, 115, 1265-1272.	2.0	16
66	Demystifying the Atomistic Origin of the Electric Field Effect on Methane Oxidation. Journal of Physical Chemistry Letters, 2020, 11, 6976-6981.	4.6	16
67	Adhesion of lubricant on aluminium through adsorption of additive head-groups on Î³-alumina: A DFT study. Tribology International, 2020, 145, 106140.	5.9	15
68	Hydroxide-Induced Degradation of Olefin Metathesis Catalysts: A Challenge for Metathesis in Alkaline Media. ACS Catalysis, 2020, 10, 3838-3843.	11.2	15
69	Autonomous high-throughput computations in catalysis. Chem Catalysis, 2022, 2, 940-956.	6.1	14
70	Study of a novel hepta-coordinated FeIII bimetallic complex with an unusual 1,2,4,5-tetrazine-ring opening. Polyhedron, 2016, 108, 163-168.	2.2	13
71	Energy Decomposition Analysis for Metal Surfaceâ€“Adsorbate Interactions by Block Localized Wave Functions. Journal of Chemical Theory and Computation, 2019, 15, 265-275.	5.3	13
72	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.	5.4	13

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73	How are small endohedral silicon clusters stabilized?. Physical Chemistry Chemical Physics, 2012, 14, 14842.	2.8	12
74	What does graphitic carbon nitride really look like?. Physical Chemistry Chemical Physics, 2021, 23, 2853-2859.	2.8	12
75	Parameter-free coordination numbers for solutions and interfaces. Journal of Chemical Physics, 2020, 152, 024124.	3.0	11
76	Nature of High- and Low-Affinity Metal Surface Sites on Birnessite Nanosheets. ACS Earth and Space Chemistry, 2021, 5, 66-76.	2.7	11
77	(Dis)Similarities of adsorption of diverse functional groups over alumina and hematite depending on the surface state. Journal of Chemical Physics, 2021, 154, 084701.	3.0	11
78	Bonding analysis of planar hypercoordinate atoms via the generalized BLWâ€ŁLOL. Journal of Computational Chemistry, 2013, 34, 2242-2248.	3.3	10
79	Water adlayers on noble metal surfaces: Insights from energy decomposition analysis. Journal of Chemical Physics, 2020, 153, 054703.	3.0	10
80	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.	3.3	9
81	Size-Dependent Structural, Energetic, and Spectroscopic Properties of MoS₃ Polymorphs. Crystal Growth and Design, 2020, 20, 7750-7760.	3.0	9
82	Transferable Gaussian Attractive Potentials for Organic/Oxide Interfaces. Journal of Physical Chemistry B, 2021, 125, 10843-10853.	2.6	8
83	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.	3.1	8
84	Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2022, 13, 6079-6084.	4.6	8
85	The Pressure Gap for Thiols: Methanethiol Self-Assembly on Au(111) from Vacuum to 1 bar. Journal of Physical Chemistry C, 2019, 123, 12382-12389.	3.1	7
86	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.	3.1	6
87	Theory and experiments join forces to characterize the electrocatalytic interface. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7611-7613.	7.1	5
88	Same ligand, three first-row metals: comparing M-amido bifunctional reactivity (Mn, Fe, Co). Dalton Transactions, 2021, 50, 14542-14546.	3.3	5
89	Genesis of MoS2 from model-Mo-oxide precursors supported on Î³-alumina. Journal of Catalysis, 2022, 408, 303-315.	6.2	4
90	Tetrazine-Based Ligand Transformation Driving Metalâ€"Metal Bond and Mixed-Valence Hg^I/Hg^{II}. ACS Omega, 2018, 3, 10273-10277.	3.5	3

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91	Strong Affinity of Triazolium-Appended Dipyrromethenes (TADs) for BF4â^'. Molecules, 2020, 25, 4555.	3.8	2
92	C6 Diacids from homocitric acid lactone using relay heterogeneous catalysis in water. Catalysis Today, 2019, 319, 191-196.	4.4	1
93	Efficient recursive least squares solver for rank-deficient matrices. Applied Mathematics and Computation, 2021, 399, 125996.	2.2	0