Matthias Stein

List of Publications by Year
in descending order

112 papers	3,529 citations	117619 34 h-index	155644 55 g-index
122 all docs	122 docs citations	122 times ranked	3474 citing authors

#	Article	IF	Citations
1	A unique iron-sulfur cluster is crucial for oxygen tolerance of a [NiFe]-hydrogenase. Nature Chemical Biology, 2011, 7, 310-318.	8.0	225
2	Single Crystal EPR Studies of the Reduced Active Site of [NiFe] Hydrogenase fromDesulfovibrio vulgarisMiyazaki F. Journal of the American Chemical Society, 2003, 125, 83-93.	13.7	196
3	Catalytic Hydrogen Evolution from Mononuclear Iron(II) Carbonyl Complexes as Minimal Functional Models of the [FeFe] Hydrogenase Active Site. Angewandte Chemie - International Edition, 2010, 49, 8033-8036.	13.8	138
4	Ligand versus Metal Protonation of an Iron Hydrogenase Active Site Mimic. Chemistry - A European Journal, 2007, 13, 7075-7084.	3.3	132
5	A Model of the [FeFe] Hydrogenase Active Site with a Biologically Relevant Azadithiolate Bridge: A Spectroscopic and Theoretical Investigation. Angewandte Chemie - International Edition, 2011, 50, 1439-1443.	13.8	130
6	Relativistic DFT Calculations of the Paramagnetic Intermediates of [NiFe] Hydrogenase. Implications for the Enzymatic Mechanism. Journal of the American Chemical Society, 2001, 123, 5839-5840.	13.7	109
7	A single-crystal ENDOR and density functional theory study of the oxidized states of the [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F. Journal of Biological Inorganic Chemistry, 2006, 11, 41-51.	2.6	103
8	webPIPSA: a web server for the comparison of protein interaction properties. Nucleic Acids Research, 2008, 36, W276-W280.	14.5	88
9	Relativistic DFT calculation of the reaction cycle intermediates of [NiFe] hydrogenase: a contribution to understanding the enzymatic mechanism. Journal of Inorganic Biochemistry, 2004, 98, 862-877.	3.5	87
10	Quantum chemical calculations of [NiFe] hydrogenase. Current Opinion in Chemical Biology, 2002, 6, 243-249.	6.1	81
11	[NiFe] hydrogenases: how close do structural and functional mimics approach the active site?. Dalton Transactions, 2014, 43, 9392.	3.3	81
12	DFT calculations of the electronic structure of the paramagnetic states Ni-A, Ni-B and Ni-C of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2001, 3, 2668-2675.	2.8	72
13	Mixed-Valence Nickelâ€“Iron Dithiolate Models of the [NiFe]-Hydrogenase Active Site. Inorganic Chemistry, 2012, 51, 2338-2348.	4.0	67
14	g- andA-Tensor Calculations in the Zero-Order Approximation for Relativistic Effects of Ni Complexes and Ni(CO)3H as Model Complexes for the Active Center of [NiFe]-Hydrogenase. Journal of Physical Chemistry A, 2001, 105, 416-425.	2.5	64
15	Isolation of a Mixed Valence Diiron Hydride: Evidence for a Spectator Hydride in Hydrogen Evolution Catalysis. Journal of the American Chemical Society, 2013, 135, 3633-3639.	13.7	63
16	Single crystal EPR studies of the oxidized active site of [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F. Journal of Biological Inorganic Chemistry, 2000, 5, 36-44.	2.6	62
17	(I,0) Mixed-Valence State of a Diiron Complex with Pertinence to the [FeFe]-Hydrogenase Active Site: An IR, EPR, and Computational Study. Inorganic Chemistry, 2009, 48, 10883-10885.	4.0	57
18	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?. Journal of the American Chemical Society, 2015, 137, 11095-11104.	13.7	57

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19	The electronic structure of the catalytic intermediate Ni-C in [NiFe] and [NiFeSe] hydrogenasesElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b105723p/. Physical Chemistry Chemical Physics, 2001, 3, 5115-5120.	2.8	55
20	Novel Enantioselective Receptors for N-Protected Glutamate and Aspartate. Chemistry - A European Journal, 2005, 11, 5674-5688.	3.3	54
21	Spectroscopic characterization of the key catalytic intermediate Niâ€“C in the O2-tolerant [NiFe] hydrogenase I from Aquifex aeolicus: evidence of a weakly bound hydride. Chemical Communications, 2012, 48, 823-825.	4.1	53
22	A theoretical study of spin states in Ni-S4 complexes and models of the [NiFe] hydrogenase active site. Journal of Biological Inorganic Chemistry, 2004, 9, 873-884.	2.6	52
23	Theoretical reassessment of Whelk-O1 as an enantioselective receptor for 1-(4-halogeno-phenyl)-1-ethylamine derivatives. Chirality, 2004, 16, S1-S11.	2.6	52
24	Direct Observation of Key Catalytic Intermediates in a Photoinduced Proton Reduction Cycle with a Diiron Carbonyl Complex. Journal of the American Chemical Society, 2014, 136, 17366-17369.	13.7	49
25	The Molecular Basis of Polyunsaturated Fatty Acid Interactions with the Shaker Voltage-Gated Potassium Channel. PLoS Computational Biology, 2016, 12, e1004704.	3.2	47
26	Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of Human Dopamine D2 Receptor Using Computational and Experimental Techniques. ACS Chemical Neuroscience, 2016, 7, 185-195.	3.5	45
27	Bridging from molecular simulation to biochemical networks. Current Opinion in Structural Biology, 2007, 17, 166-172.	5.7	44
28	Accurate Calculations of Ligand Binding Free Energies:Â Chiral Separation with Enantioselective Receptors. Journal of Physical Chemistry A, 2004, 108, 3572-3580.	2.5	43
29	Facilitated Hydride Binding in an Feâ^'Fe Hydrogenase Activeâ^'Site Biomimic Revealed by X-ray Absorption Spectroscopy and DFT Calculations. Inorganic Chemistry, 2007, 46, 11094-11105.	4.0	43
30	Coordination and conformational isomers in mononuclear iron complexes with pertinence to the [FeFe] hydrogenase active site. Dalton Transactions, 2014, 43, 4537-4549.	3.3	43
31	Connecting [NiFe]- and [FeFe]-Hydrogenases: Mixed-Valence Nickelâ€“Iron Dithiolates with Rotated Structures. Inorganic Chemistry, 2012, 51, 8931-8941.	4.0	41
32	Design, Synthesis and Biological Evaluation of Sugar-Derived Ras Inhibitors. ChemBioChem, 2005, 6, 1839-1848.	2.6	39
33	qPIPSA: Relating enzymatic kinetic parameters and interaction fields. BMC Bioinformatics, 2007, 8, 373.	2.6	38
34	The Interaction Properties of the Human Rab GTPase Family â€“ A Comparative Analysis Reveals Determinants of Molecular Binding Selectivity. PLoS ONE, 2012, 7, e34870.	2.5	38
35	In Situ Infrared Spectroscopy as a Tool for Monitoring Molecular Catalyst for Hydroformylation in Continuous Processes. ACS Catalysis, 2019, 9, 4308-4319.	11.2	35
36	[NiFe] and [FeS] Cofactors in the Membrane-Bound Hydrogenase of Ralstonia eutropha Investigated by X-ray Absorption Spectroscopy: Insights into O₂-Tolerant H₂ Cleavage. Biochemistry, 2011, 50, 5858-5869.	2.5	33

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37	Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 4676-4686.	3.0	33
38	SYCAMOREâ€”a <u>sy</u>stems biology <u>c</u>omputational <u>a</u>nalysis and <u>mo</u>deling <u>r</u>esearch <u>e</u>nvironment. Bioinformatics, 2008, 24, 1463-1464.	4.1	31
39	Design, Synthesis, and Biological Evaluation of LevoglucosenoneâEDerived Ras Activation Inhibitors. ChemMedChem, 2009, 4, 524-528.	3.2	31
40	Orientation-selected ENDOR of the active center in Chromatium vinosum [NiFe] hydrogenase in the oxidized "ready" state. Journal of Biological Inorganic Chemistry, 1999, 4, 379-389.	2.6	30
41	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. Molecular Diversity, 2015, 19, 321-332.	3.9	29
42	Ni^I/Ru^{II} Model for the Niâ€“L State of the [NiFe]Hydrogenases: Synthesis, Spectroscopy, and Reactivity. Inorganic Chemistry, 2014, 53, 4243-4249.	4.0	28
43	Targeting the NF-ÎºB/IÎºBÎ± complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models. Journal of Molecular Graphics and Modelling, 2019, 86, 264-277.	2.4	28
44	Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking. ACS Chemical Neuroscience, 2017, 8, 1404-1415.	3.5	23
45	Membrane localization and dynamics of geranylgeranylated Rab5 hypervariable region. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1335-1349.	2.6	18
46	Molecular Reorganization Energy as a Key Determinant of J-Band Formation in J-Aggregates of Polymethine Dyes. Journal of Physical Chemistry A, 2015, 119, 6773-6780.	2.5	17
47	The thermodynamics and biodegradability of chelating agents upon metal extraction. Chemical Engineering Science, 2015, 137, 768-785.	3.8	17
48	A mononuclear iron carbonyl complex [Fe(Î¼-bdt)(CO)₂(PTA)₂] with bulky phosphine ligands: a model for the [FeFe] hydrogenase enzyme active site with an inverted redox potential. Dalton Transactions, 2017, 46, 10050-10056.	3.3	17
49	Molecular Dynamics Study of the Solution Structure, Clustering, and Diffusion of Four Aqueous Alkanolamines. Journal of Physical Chemistry B, 2018, 122, 2769-2778.	2.6	17
50	Computational Studies on the Inhibitor Selectivity of Human JAMM Deubiquitinylases Rpn11 and CSN5. Frontiers in Chemistry, 2018, 6, 480.	3.6	17
51	Cross-species analysis of the glycolytic pathway by comparison of molecular interaction fields. Molecular BioSystems, 2009, 6, 162-174.	2.9	16
52	Intramolecular stabilization of a catalytic [FeFe]-hydrogenase mimic investigated by experiment and theory. Dalton Transactions, 2018, 47, 4941-4949.	3.3	16
53	Intermolecular Interactions in Molecular Organic Crystals upon Relaxation of Lattice Parameters. Crystals, 2019, 9, 665.	2.2	16
54	Effect of Cyanide Ligands on the Electronic Structure of [FeFe] Hydrogenase Activeâ€Site Model Complexes with an Azadithiolate Cofactor. Chemistry - A European Journal, 2013, 19, 14566-14572.	3.3	15

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55	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ACS Chemical Neuroscience, 2017, 8, 826-836.	3.5	15
56	Solvent Selection in Homogeneous Catalysisâ€"Optimization of Kinetics and Reaction Performance. ACS Catalysis, 2021, 11, 590-594.	11.2	15
57	Probing the druggability of membrane-bound Rab5 by molecular dynamics simulations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 434-443.	5.2	14
58	Predicting solvent effects on the 1â€dodecene hydroformylation reaction equilibrium. AICHE Journal, 2017, 63, 4576-4585.	3.6	14
59	Accurate lattice energies of organic molecular crystals from periodic turbomole calculations. Journal of Computational Chemistry, 2018, 39, 1335-1343.	3.3	14
60	The effect of CO₂ loading on alkanolamine absorbents in aqueous solutions. Physical Chemistry Chemical Physics, 2019, 21, 18386-18392.	2.8	14
61	Chemicalâ€Shift Perturbations Reflect Bile Acid Binding to Norovirus Coat Protein: Recognition Comes in Different Flavors. ChemBioChem, 2020, 21, 1007-1021.	2.6	14
62	Activation and selectivity of OTUB-1 and OTUB-2 deubiquitinylases. Journal of Biological Chemistry, 2020, 295, 6972-6982.	3.4	14
63	Accurate Receptor-Ligand Binding Free Energies from Fast QM Conformational Chemical Space Sampling. International Journal of Molecular Sciences, 2021, 22, 3078.	4.1	14
64	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2040-2048.	3.5	13
65	Mechanism and Control of the Palladiumâ€Catalyzed Alkoxycarbonylation of Oleochemicals from Sustainable Sources. ChemCatChem, 2019, 11, 4894-4906.	3.7	13
66	Restricted rotation of an Fe(CO)₂(PL₃)-subunit in [FeFe]-hydrogenase active site mimics by intramolecular ligation. Dalton Transactions, 2019, 48, 5933-5939.	3.3	13
67	Modulation of Jahnâ€"Teller distortion and electromechanical response in a Mn³⁺ spin crossover complex. Journal of Physics Condensed Matter, 2020, 32, 404002.	1.8	13
68	Spin-State-Dependent Properties of an Iron(III) Hydrogenase Mimic. European Journal of Inorganic Chemistry, 2014, 2014, 3587-3599.	2.0	12
69	Simulation of Mixed Self-Assembled Monolayers on Gold: Effect of Terminal Alkyl Anchor Chain and Monolayer Composition. Journal of Physical Chemistry B, 2018, 122, 7699-7710.	2.6	12
70	Kinetics of the reductive amination of 1-undecanal in thermomorphic multicomponent system. Chemical Engineering Science, 2021, 230, 116187.	3.8	12
71	Mn(III) complexes with nitro-substituted ligandsâ€"Spin states with a twist. Journal of Applied Physics, 2021, 129, .	2.5	12
72	Incorporation of Î²â€Alanine in Cu(II) ATCUN Peptide Complexes Increases ROS Levels, DNA Cleavage and Antiproliferative Activity**. Chemistry - A European Journal, 2021, 27, 18093-18102.	3.3	12

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73	Proteinâ€“Protein Complex Formation Affects the Niâ€“Fe and Feâ€“S Centers in the H₂â€Sensing Regulatory Hydrogenase from Ralstonia eutropha H16. ChemPhysChem, 2010, 11, 1297-1306.	2.1	11
74	Rates and Routes of Electron Transfer of [NiFe]-Hydrogenase in an Enzymatic Fuel Cell. Journal of Physical Chemistry B, 2015, 119, 13870-13882.	2.6	11
75	Resolution of structural isomers of complex reaction mixtures in homogeneous catalysis. Chemical Engineering and Processing: Process Intensification, 2016, 102, 229-237.	3.6	11
76	Diversity in a simple co-crystal: racemic and kryptoracemic behaviour. Chemical Communications, 2016, 52, 8309-8312.	4.1	11
77	Solvation and Dynamics of CO₂ in Aqueous Alkanolamine Solutions. ACS Sustainable Chemistry and Engineering, 2019, 7, 1028-1037.	6.7	11
78	Ovarian tumor domain proteases in pathogen infection. Trends in Microbiology, 2022, 30, 22-33.	7.7	11
79	EPR and ENDOR Studies of [NiFe] Hydrogenase: Contributions to Understanding the Mechanism of Biological Hydrogen Conversion. ACS Symposium Series, 2003, , 128-149.	0.5	10
80	The thermochemistry of long chain olefin isomers during hydroformylation. New Journal of Chemistry, 2017, 41, 7347-7355.	2.8	10
81	Distal [FeS]-Cluster Coordination in [NiFe]-Hydrogenase Facilitates Intermolecular Electron Transfer. International Journal of Molecular Sciences, 2017, 18, 100.	4.1	10
82	Double phosphorylationâ€induced structural changes in the signalâ€receiving domain of IÎºBÎ± in complex with NFâ€ÎºB. Proteins: Structure, Function and Bioinformatics, 2017, 85, 17-29.	2.6	9
83	Modelling the photonucleation of water vapour by UV in the presence of oxygen and the absence of pollutants. Faraday Discussions, 1995, 100, 253.	3.2	8
84	Calculating enzyme kinetic parameters from protein structures. Biochemical Society Transactions, 2008, 36, 51-54.	3.4	8
85	Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst. RSC Advances, 2018, 8, 36662-36674.	3.6	8
86	The many roles of solvent in homogeneous catalysis - The reductive amination showcase. Journal of Catalysis, 2022, 405, 24-34.	6.2	8
87	QM/MM Investigation of the Role of a Second Coordination Shell Arginine in [NiFe]-Hydrogenases. Frontiers in Chemistry, 2018, 6, 164.	3.6	7
88	A QM proteinâ€“ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). Journal of Biomolecular Structure and Dynamics, 2018, 36, 2668-2677.	3.5	6
89	Structure and Dynamics of Mono- vs. Doubly Lipidated Rab5 in Membranes. International Journal of Molecular Sciences, 2019, 20, 4773.	4.1	6
90	Toward a Molecular Reorganization Energy-Based Analysis of Third-Order Nonlinear Optical Properties of Polymethine Dyes and J-Aggregates. Journal of Physical Chemistry A, 2019, 123, 9321-9327.	2.5	6

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91	Switching Site Reactivity in Hydrogenase Model Systems by Introducing a Pendant Amine Ligand. ACS Omega, 2021, 6, 4192-4203.	3.5	6
92	Binding of SARS-CoV Covalent Non-Covalent Inhibitors to the SARS-CoV-2 Papain-Like Protease and Ovarian Tumor Domain Deubiquitinases. Biomolecules, 2021, 11, 802.	4.0	6
93	Mechanism of Diiron Hydrogenase Complexes Controlled by Nature of Bridging Dithiolate Ligand. ChemistryOpen, 2022, 11, e202100238.	1.9	6
94	Structural modeling of the N-terminal signalâ€“receiving domain of IÎºBÎ±. Frontiers in Molecular Biosciences, 2015, 2, 32.	3.5	5
95	Regularization of Poisson–Boltzmann Type Equations with Singular Source Terms Using the Range-Separated Tensor Format. SIAM Journal of Scientific Computing, 2021, 43, A415-A445.	2.8	5
96	Recognition and stabilization of geranylgeranylated human Rab5 by the GDP Dissociation Inhibitor (GDI). Small GTPases, 2019, 10, 227-242.	1.6	4
97	Solvent effects in hydroformylation of long-chain olefins. Molecular Catalysis, 2021, 503, 111429.	2.0	4
98	<scp>Substrateâ€assisted</scp> activation and selectivity of the bacterial <scp>RavD</scp> effector deubiquitinylase. Proteins: Structure, Function and Bioinformatics, 2022, 90, 947-958.	2.6	4
99	EPR and theoretical investigations of [NiFe] hydrogenase: Insight into the mechanism of biological hydrogen conversion. , 2002, , 437-445.		3
100	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2HighR and D2LowR States. Journal of Chemical Information and Modeling, 2018, 58, 826-836.	5.4	3
101	Fast solution of the linearized Poissonâ€“Boltzmann equation with nonaffine parametrized boundary conditions using the reduced basis method. Computing and Visualization in Science, 2020, 23, 1.	1.2	3
102	The Activation and Selectivity of the Legionella RavD Deubiquitinase. Frontiers in Molecular Biosciences, 2021, 8, 770320.	3.5	3
103	Comment on â€œA Nickel(II)â€Based Radicalâ€Ligand Complex as a Functional Model of Hydrogenaseâ€. Chemistry - A European Journal, 2011, 17, 15046-15048.	3.3	2
104	Microbial hydrogen splitting in the presence of oxygen. Biochemical Society Transactions, 2013, 41, 1317-1324.	3.4	2
105	VIBRATIONAL SCALING FACTORS FOR Rh(I) CARBONYL COMPOUNDS IN HOMOGENEOUS CATALYSIS. Prilozi: Makedonska Akademija Na Naukite I Umetnostite Oddelenie Za Prirodno-matematiÄki I BiotehniÄki Nauki, 2017, 38, 43.	0.3	2
106	REDUCED BASIS METHOD FOR POISSON-BOLTZMANN EQUATION. , 2016, , .		2
107	Reduced basis method for the nonlinear Poissonâ€“Boltzmann equation regularized by the range-separated canonical tensor format. International Journal of Nonlinear Sciences and Numerical Simulation, 2024, 24, 2915-2935.	1.0	2
108	Molecular Characterization of the Binding of Polyunsaturated Fatty Acids to a Voltage-Gated Potassium Channel. Biophysical Journal, 2014, 106, 739a.	0.5	0

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109	Vorhersage des LÃ¶sungsmitteleinflusses auf das Reaktionsgleichgewicht der Hydroformylierung von 1-Dodecen. Chemie-Ingenieur-Technik, 2016, 88, 1382-1383.	0.8	0
110	Correction to Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 6149-6149.	3.0	0
111	Cover Image, Volume 85, Issue 1. Proteins: Structure, Function and Bioinformatics, 2017, 85, C4.	2.6	0
112	Anisotropic Magnetic Spin Interactions of Transition Metal Complexes and Metalloenzymes from Spectroscopy and Quantum Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2019, , 35-64.	0.6	0