Martin J Field

List of Publications by Year
in descending order

41 papers	5,261 citations	218677 26 h-index	289244 40 g-index
41 all docs	41 docs citations	41 times ranked	4325 citing authors

#	Article	IF	Citations
1	Modeling the Hydrolysis of Ironâ€“Sulfur Clusters. Journal of Chemical Information and Modeling, 2020, 60, 653-660.	5.4	12
2	Electrocatalytic Hydrogen Evolution with a Cobalt Complex Bearing Pendant Proton Relays: Acid Strength and Applied Potential Govern Mechanism and Stability. Journal of the American Chemical Society, 2020, 142, 274-282.	13.7	92
3	Photoswitching mechanism of a fluorescent protein revealed by time-resolved crystallography and transient absorption spectroscopy. Nature Communications, 2020, 11, 741.	12.8	56
4	Chromophore twisting in the excited state of a photoswitchable fluorescent protein captured by time-resolved serial femtosecond crystallography. Nature Chemistry, 2018, 10, 31-37.	13.6	152
5	Protonâ€Reduction Reaction Catalyzed by Homoleptic Nickelâ€“bisâ€1,2â€dithiolate Complexes: Experimental and Theoretical Mechanistic Investigations. ChemCatChem, 2017, 9, 2308-2317.	3.7	50
6	An Algorithm for Adaptive QC/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2342-2351.	5.3	27
7	Norovirus RNAâ€dependent RNA polymerase: A computational study of metalâ€binding preferences. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1435-1445.	2.6	10
8	Catalytic Mechanism of Peptidoglycan Deacetylase: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 89-99.	2.6	2
9	Experimental and Theoretical Insight into Electrocatalytic Hydrogen Evolution with Nickel Bis(aryldithiolene) Complexes as Catalysts. Inorganic Chemistry, 2016, 55, 432-444.	4.0	76
10	Force-induced chemical reactions on the metal centre in a single metalloprotein molecule. Nature Communications, 2015, 6, 7569.	12.8	33
11	Technical advances in molecular simulation since the 1980s. Archives of Biochemistry and Biophysics, 2015, 582, 3-9.	3.0	12
12	Pcetk: A pDynamo-based Toolkit for Protonation State Calculations in Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2288-2296.	5.4	6
13	Ferricâ€“Thiolate Bond Dissociation Studied with Electronic Structure Calculations. Journal of Physical Chemistry A, 2015, 119, 10084-10090.	2.5	12
14	Multiscale modeling of nerve agent hydrolysis mechanisms: a tale of two Nobel Prizes. Physica Scripta, 2014, 89, 108004.	2.5	13
15	Characterization of the divalent metal binding site of bacterial polysaccharide deacetylase using crystallography and quantum chemical calculations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1311-1318.	2.6	2
16	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. Israel Journal of Chemistry, 2014, 54, 1250-1263.	2.3	45
17	Electronic Structure and Hydration of Tetramine Cobalt Hydride Complexes. Journal of Physical Chemistry B, 2014, 118, 5551-5561.	2.6	10
18	Theoretical Modeling of Lowâ€Energy Electronic Absorption Bands in Reduced Cobaloximes. ChemPhysChem, 2014, 15, 2951-2958.	2.1	11

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19	Cobaloxime-Based Artificial Hydrogenases. Inorganic Chemistry, 2014, 53, 8071-8082.	4.0	78
20	Homolytic Cleavage of Feï£¿S Bonds in Rubredoxin under Mechanical Stress. Angewandte Chemie - International Edition, 2013, 52, 8144-8146.	13.8	23
21	A Computational Study of the Mechanism of Hydrogen Evolution by Cobalt(Diimineâ€Dioxime) Catalysts. Chemistry - A European Journal, 2013, 19, 15166-15174.	3.3	91
22	Catalytic hydrogen production by a Niâ€"Ru mimic of NiFe hydrogenases involves a proton-coupled electron transfer step. Chemical Communications, 2013, 49, 5004.	4.1	54
23	A hybrid elastic band string algorithm for studies of enzymatic reactions. Physical Chemistry Chemical Physics, 2012, 14, 12544.	2.8	21
24	Combined Experimentalâ€"Theoretical Characterization of the Hydrido-Cobaloxime [HCo(dmgH)₂(PnBu₃)]. Inorganic Chemistry, 2012, 51, 7087-7093.	4.0	55
25	A nickelâ€"manganese catalyst as a biomimic of the active site of NiFe hydrogenases: a combined electrocatalytical and DFT mechanistic study. Energy and Environmental Science, 2011, 4, 2417.	30.8	85
26	Mechanism of hydrogen evolution catalyzed by NiFe hydrogenases: insights from a Niâ€"Ru model compound. Dalton Transactions, 2010, 39, 3043-3049.	3.3	39
27	A structural and functional mimic of the active site of NiFe hydrogenases. Chemical Communications, 2010, 46, 5876.	4.1	101
28	Cyclopentadienyl Rutheniumâ€"Nickel Catalysts for Biomimetic Hydrogen Evolution: Electrocatalytic Properties and Mechanistic DFT Studies. Chemistry - A European Journal, 2009, 15, 9350-9364.	3.3	61
29	Improving the efficiency of the NEB reaction path finding algorithm. Journal of Computational Chemistry, 2008, 29, 139-143.	3.3	30
30	The pDynamo Program for Molecular Simulations using Hybrid Quantum Chemical and Molecular Mechanical Potentials. Journal of Chemical Theory and Computation, 2008, 4, 1151-1161.	5.3	99
31	Structural characterization of IrisFP, an optical highlighter undergoing multiple photo-induced transformations. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 18343-18348.	7.1	211
32	Simulating enzyme reactions: Challenges and perspectives. Journal of Computational Chemistry, 2002, 23, 48-58.	3.3	177
33	The dynamo library for molecular simulations using hybrid quantum mechanical and molecular mechanical potentials. Journal of Computational Chemistry, 2000, 21, 1088-1100.	3.3	293
34	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. Theoretical Chemistry Accounts, 2000, 104, 336-343.	1.4	110
35	A Generalized Hybrid Orbital (GHO) Method for the Treatment of Boundary Atoms in Combined QM/MM Calculations. Journal of Physical Chemistry A, 1998, 102, 4714-4721.	2.5	481
36	Hybrid quantum mechanical/molecular mechanical fluctuating charge models for condensed phase simulations. Molecular Physics, 1997, 91, 835-845.	1.7	54

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37	Report for the joint CECAM-NSF planning meeting on hybrid quantum and classical mechanical methods for the simulation of biopolymers in solution (May 9-11, 1995). International Journal of Quantum Chemistry, 1996, 60, 1093-1096.	2.0	2
38	Simulation analysis of triose phosphate isomerase: conformational transition and catalysis. Faraday Discussions, 1992, 93, 239.	3.2	39
39	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. Journal of Computational Chemistry, 1990, 11, 700-733.	3.3	2,230
40	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. , 1990, 11, 700.		1
41	Free energy perturbation method for chemical reactions in the condensed phase: a dynamic approach based on a combined quantum and molecular mechanics potential. Journal of the American Chemical Society, 1987, 109, 8092-8094.	13.7	305