Martin J Field

List of Publications by Year in descending order

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41 papers	5,261 citations	218381 26 h-index	288905 40 g-index
41 all docs	41 docs citations	41 times ranked	4325 citing authors

#	Article	IF	Citations
1	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. Journal of Computational Chemistry, 1990, 11, 700-733.	1.5	2,230
2	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.	1.1	481
3	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.	6.6	305
4	The dynamo library for molecular simulations using hybrid quantum mechanical and molecular mechanical potentials. Journal of Computational Chemistry, 2000, 21, 1088-1100.	1.5	293
5	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.	3.3	211
6	Simulating enzyme reactions: Challenges and perspectives. Journal of Computational Chemistry, 2002, 23, 48-58.	1.5	177
7	Chromophore twisting in the excited state of a photoswitchable fluorescent protein captured by time-resolved serial femtosecond crystallography. Nature Chemistry, 2018, 10, 31-37.	6.6	152
8	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.	0.5	110
9	A structural and functional mimic of the active site of NiFe hydrogenases. Chemical Communications, 2010, 46, 5876.	2.2	101
10	The pDynamo Program for Molecular Simulations using Hybrid Quantum Chemical and Molecular Mechanical Potentials. Journal of Chemical Theory and Computation, 2008, 4, 1151-1161.	2.3	99
11	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.	6.6	92
12	A Computational Study of the Mechanism of Hydrogen Evolution by Cobalt(Diimineâ€Dioxime) Catalysts. Chemistry - A European Journal, 2013, 19, 15166-15174.	1.7	91
13	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.	15.6	85
14	Cobaloxime-Based Artificial Hydrogenases. Inorganic Chemistry, 2014, 53, 8071-8082.	1.9	78
15	Experimental and Theoretical Insight into Electrocatalytic Hydrogen Evolution with Nickel Bis(aryldithiolene) Complexes as Catalysts. Inorganic Chemistry, 2016, 55, 432-444.	1.9	76
16	Cyclopentadienyl Rutheniumâ€“Nickel Catalysts for Biomimetic Hydrogen Evolution: Electrocatalytic Properties and Mechanistic DFT Studies. Chemistry - A European Journal, 2009, 15, 9350-9364.	1.7	61
17	Photoswitching mechanism of a fluorescent protein revealed by time-resolved crystallography and transient absorption spectroscopy. Nature Communications, 2020, 11, 741.	5.8	56
18	Combined Experimentalâ€“Theoretical Characterization of the Hydrido-Cobaloxime [HCo(dmgH)₂(PnBu₃)]. Inorganic Chemistry, 2012, 51, 7087-7093.	1.9	55

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19	Catalytic hydrogen production by a Niâ€“Ru mimic of NiFe hydrogenases involves a proton-coupled electron transfer step. Chemical Communications, 2013, 49, 5004.	2.2	54
20	Hybrid quantum mechanical/molecular mechanical fluctuating charge models for condensed phase simulations. Molecular Physics, 1997, 91, 835-845.	0.8	54
21	Protonâ€Reduction Reaction Catalyzed by Homoleptic Nickelâ€“bisâ€1,2â€dithiolate Complexes: Experimental and Theoretical Mechanistic Investigations. ChemCatChem, 2017, 9, 2308-2317.	1.8	50
22	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. Israel Journal of Chemistry, 2014, 54, 1250-1263.	1.0	45
23	Simulation analysis of triose phosphate isomerase: conformational transition and catalysis. Faraday Discussions, 1992, 93, 239.	1.6	39
24	Mechanism of hydrogen evolution catalyzed by NiFe hydrogenases: insights from a Niâ€“Ru model compound. Dalton Transactions, 2010, 39, 3043-3049.	1.6	39
25	Force-induced chemical reactions on the metal centre in a single metalloprotein molecule. Nature Communications, 2015, 6, 7569.	5.8	33
26	Improving the efficiency of the NEB reaction path finding algorithm. Journal of Computational Chemistry, 2008, 29, 139-143.	1.5	30
27	An Algorithm for Adaptive QC/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2342-2351.	2.3	27
28	Homolytic Cleavage of Feï¿¿S Bonds in Rubredoxin under Mechanical Stress. Angewandte Chemie - International Edition, 2013, 52, 8144-8146.	7.2	23
29	A hybrid elastic band string algorithm for studies of enzymatic reactions. Physical Chemistry Chemical Physics, 2012, 14, 12544.	1.3	21
30	Multiscale modeling of nerve agent hydrolysis mechanisms: a tale of two Nobel Prizes. Physica Scripta, 2014, 89, 108004.	1.2	13
31	Technical advances in molecular simulation since the 1980s. Archives of Biochemistry and Biophysics, 2015, 582, 3-9.	1.4	12
32	Ferricâ€“Thiolate Bond Dissociation Studied with Electronic Structure Calculations. Journal of Physical Chemistry A, 2015, 119, 10084-10090.	1.1	12
33	Modeling the Hydrolysis of Ironâ€“Sulfur Clusters. Journal of Chemical Information and Modeling, 2020, 60, 653-660.	2.5	12
34	Theoretical Modeling of Lowâ€Energy Electronic Absorption Bands in Reduced Cobaloximes. ChemPhysChem, 2014, 15, 2951-2958.	1.0	11
35	Electronic Structure and Hydration of Tetramine Cobalt Hydride Complexes. Journal of Physical Chemistry B, 2014, 118, 5551-5561.	1.2	10
36	Norovirus RNAâ€dependent RNA polymerase: A computational study of metalâ€binding preferences. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1435-1445.	1.5	10

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37	Pcetk: A pDynamo-based Toolkit for Protonation State Calculations in Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2288-2296.	2.5	6
38	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.	1.0	2
39	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.	1.5	2
40	Catalytic Mechanism of Peptidoglycan Deacetylase: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 89-99.	1.2	2
41	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. , 1990, 11, 700.		1