

Martin J Field

List of Publications by Year in descending order

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41
papers

5,261
citations

218677
26
h-index

289244
40
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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. <i>Journal of Computational Chemistry</i> , 1990, 11, 700-733.	3.3	2,230
2	A Generalized Hybrid Orbital (GHO) Method for the Treatment of Boundary Atoms in Combined QM/MM Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4714-4721.	2.5	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. <i>Journal of the American Chemical Society</i> , 1987, 109, 8092-8094.	13.7	305
4	The dynamo library for molecular simulations using hybrid quantum mechanical and molecular mechanical potentials. <i>Journal of Computational Chemistry</i> , 2000, 21, 1088-1100.	3.3	293
5	Structural characterization of IrisFP, an optical highlighter undergoing multiple photo-induced transformations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 18343-18348.	7.1	211
6	Simulating enzyme reactions: Challenges and perspectives. <i>Journal of Computational Chemistry</i> , 2002, 23, 48-58.	3.3	177
7	Chromophore twisting in the excited state of a photoswitchable fluorescent protein captured by time-resolved serial femtosecond crystallography. <i>Nature Chemistry</i> , 2018, 10, 31-37.	13.6	152
8	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 336-343.	1.4	110
9	A structural and functional mimic of the active site of NiFe hydrogenases. <i>Chemical Communications</i> , 2010, 46, 5876.	4.1	101
10	The pDynamo Program for Molecular Simulations using Hybrid Quantum Chemical and Molecular Mechanical Potentials. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1151-1161.	5.3	99
11	Electrocatalytic Hydrogen Evolution with a Cobalt Complex Bearing Pendant Proton Relays: Acid Strength and Applied Potential Govern Mechanism and Stability. <i>Journal of the American Chemical Society</i> , 2020, 142, 274-282.	13.7	92
12	A Computational Study of the Mechanism of Hydrogen Evolution by Cobalt(Diimine- \rightarrow Dioxime) Catalysts. <i>Chemistry - A European Journal</i> , 2013, 19, 15166-15174.	3.3	91
13	A nickel- \rightarrow manganese catalyst as a biomimic of the active site of NiFe hydrogenases: a combined electrocatalytic and DFT mechanistic study. <i>Energy and Environmental Science</i> , 2011, 4, 2417.	30.8	85
14	Cobaloxime-Based Artificial Hydrogenases. <i>Inorganic Chemistry</i> , 2014, 53, 8071-8082.	4.0	78
15	Experimental and Theoretical Insight into Electrocatalytic Hydrogen Evolution with Nickel Bis(aryldithiolene) Complexes as Catalysts. <i>Inorganic Chemistry</i> , 2016, 55, 432-444.	4.0	76
16	Cyclopentadienyl Ruthenium- \rightarrow Nickel Catalysts for Biomimetic Hydrogen Evolution: Electrocatalytic Properties and Mechanistic DFT Studies. <i>Chemistry - A European Journal</i> , 2009, 15, 9350-9364.	3.3	61
17	Photoswitching mechanism of a fluorescent protein revealed by time-resolved crystallography and transient absorption spectroscopy. <i>Nature Communications</i> , 2020, 11, 741.	12.8	56
18	Combined Experimental- \rightarrow Theoretical Characterization of the Hydrido-Cobaloxime $[\text{HCo}(\text{dmgh})_2(\text{P}^n\text{Bu}_3)]$. <i>Inorganic Chemistry</i> , 2012, 51, 7087-7093.	4.0	55

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19	Catalytic hydrogen production by a Ni–Ru mimic of NiFe hydrogenases involves a proton-coupled electron transfer step. <i>Chemical Communications</i> , 2013, 49, 5004.	4.1	54
20	Hybrid quantum mechanical/molecular mechanical fluctuating charge models for condensed phase simulations. <i>Molecular Physics</i> , 1997, 91, 835-845.	1.7	54
21	Proton–Reduction Reaction Catalyzed by Homoleptic Nickel–bis(1,2-ethanedithiolate) Complexes: Experimental and Theoretical Mechanistic Investigations. <i>ChemCatChem</i> , 2017, 9, 2308-2317.	3.7	50
22	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. <i>Israel Journal of Chemistry</i> , 2014, 54, 1250-1263.	2.3	45
23	Simulation analysis of triose phosphate isomerase: conformational transition and catalysis. <i>Faraday Discussions</i> , 1992, 93, 239.	3.2	39
24	Mechanism of hydrogen evolution catalyzed by NiFe hydrogenases: insights from a Ni–Ru model compound. <i>Dalton Transactions</i> , 2010, 39, 3043-3049.	3.3	39
25	Force-induced chemical reactions on the metal centre in a single metalloprotein molecule. <i>Nature Communications</i> , 2015, 6, 7569.	12.8	33
26	Improving the efficiency of the NEB reaction path finding algorithm. <i>Journal of Computational Chemistry</i> , 2008, 29, 139-143.	3.3	30
27	An Algorithm for Adaptive QC/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2342-2351.	5.3	27
28	Homolytic Cleavage of Fe–S Bonds in Rubredoxin under Mechanical Stress. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 8144-8146.	13.8	23
29	A hybrid elastic band string algorithm for studies of enzymatic reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12544.	2.8	21
30	Multiscale modeling of nerve agent hydrolysis mechanisms: a tale of two Nobel Prizes. <i>Physica Scripta</i> , 2014, 89, 108004.	2.5	13
31	Technical advances in molecular simulation since the 1980s. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 3-9.	3.0	12
32	Ferric–Thiolate Bond Dissociation Studied with Electronic Structure Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10084-10090.	2.5	12
33	Modeling the Hydrolysis of Iron–Sulfur Clusters. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 653-660.	5.4	12
34	Theoretical Modeling of Low–Energy Electronic Absorption Bands in Reduced Cobaloximes. <i>ChemPhysChem</i> , 2014, 15, 2951-2958.	2.1	11
35	Electronic Structure and Hydration of Tetramine Cobalt Hydride Complexes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5551-5561.	2.6	10
36	Norovirus RNA–dependent RNA polymerase: A computational study of metal-binding preferences. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1435-1445.	2.6	10

#	ARTICLE	IF	CITATIONS
37	<i>Pcetk</i> : A pDynamo-based Toolkit for Protonation State Calculations in Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2288-2296.	5.4	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.	2.0	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.	2.6	2
40	Catalytic Mechanism of Peptidoglycan Deacetylase: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 89-99.	2.6	2
41	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. , 1990, 11, 700.		1