Per E M Siegbahn

List of Publications by Year
in descending order

218 papers	16,821 citations	11651 70 h-index	18130 120 g-index
225 all docs	225 docs citations	225 times ranked	9358 citing authors

#	Article	IF	Citations
1	A New Intermolecular Interaction:â€‰UnconventionalHydrogen Bonds with Elementâ€“Hydride Bonds as ProtonAcceptor. Accounts of Chemical Research, 1996, 29, 348-354.	15.6	639
2	Transition-Metal Systems in Biochemistry Studied by High-Accuracy Quantum Chemical Methods. Chemical Reviews, 2000, 100, 421-438.	47.7	559
3	Quantum Chemical Studies of Mechanisms for Metalloenzymes. Chemical Reviews, 2014, 114, 3601-3658.	47.7	494
4	Hydration of Beryllium, Magnesium, Calcium, and Zinc Ions Using Density Functional Theory. Journal of Physical Chemistry A, 1998, 102, 219-228.	2.5	487
5	Structures and Energetics for O₂ Formation in Photosystem II. Accounts of Chemical Research, 2009, 42, 1871-1880.	15.6	485
6	Computational Studies of [NiFe] and [FeFe] Hydrogenases. Chemical Reviews, 2007, 107, 4414-4435.	47.7	383
7	Water oxidation mechanism in photosystem II, including oxidations, proton release pathways, Oâ€•O bond formation and O2 release. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 1003-1019.	1.0	335
8	Mechanism of Câ€™H Activation by Diiron Methane Monooxygenases:Â Quantum Chemical Studies. Journal of the American Chemical Society, 1997, 119, 3103-3113.	13.7	302
9	Modeling Enzymatic Reactions Involving Transition Metals. Accounts of Chemical Research, 2006, 39, 729-738.	15.6	301
10	Manganese Oxyl Radical Intermediates and Oâ€™O Bond Formation in Photosynthetic Oxygen Evolution and a Proposed Role for the Calcium Cofactor in Photosystem II. Journal of the American Chemical Society, 1999, 121, 117-127.	13.7	276
11	Quantum Chemical Studies of Radical-Containing Enzymes. Chemical Reviews, 2003, 103, 2421-2456.	47.7	266
12	Recent developments of the quantum chemical cluster approach for modeling enzyme reactions. Journal of Biological Inorganic Chemistry, 2009, 14, 643-651.	2.6	257
13	DENSITYFUNCTIONALTHEORY OFBIOLOGICALLYRELEVANTMETALCENTERS. Annual Review of Physical Chemistry, 1999, 50, 221-249.	10.8	250
14	The performance of hybrid DFT for mechanisms involving transition metal complexes in enzymes. Journal of Biological Inorganic Chemistry, 2006, 11, 695-701.	2.6	237
15	Quantifying the effects of the self-interaction error in DFT: When do the delocalized states appear?. Journal of Chemical Physics, 2005, 122, 224103.	3.0	230
16	Electrocatalytic Water Oxidation by a Dinuclear Copper Complex in a Neutral Aqueous Solution. Angewandte Chemie - International Edition, 2015, 54, 4909-4914.	13.8	228
17	Oï¿¿O Bond Formation in the S4 State of the Oxygen-Evolving Complex in Photosystem II. Chemistry - A European Journal, 2006, 12, 9217-9227.	3.3	226
18	A Structureâ€Consistent Mechanism for Dioxygen Formation in Photosystem II. Chemistry - A European Journal, 2008, 14, 8290-8302.	3.3	215

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19	Modeling Electron Transfer in Biochemistry:â€‰ A Quantum Chemical Study of Charge Separation in Rhodobacter sphaeroides and Photosystem II. Journal of the American Chemical Society, 1998, 120, 8812-8824.	13.7	207
20	Quantum Chemical Studies of Proton-Coupled Electron Transfer in Metalloenzymes. Chemical Reviews, 2010, 110, 7040-7061.	47.7	186
21	Significant van der Waals Effects in Transition Metal Complexes. Journal of Chemical Theory and Computation, 2010, 6, 2040-2044.	5.3	185
22	Mechanism of Hâ‚‚ Activation by Nickelâ€“Iron Hydrogenase. Journal of the American Chemical Society, 1998, 120, 548-555.	13.7	173
23	Mechanisms of metalloenzymes studied by quantum chemical methods. Quarterly Reviews of Biophysics, 2003, 36, 91-145.	5.7	171
24	Theoretical Models for the Oxygen Radical Mechanism of Water Oxidation and of the Water Oxidizing Complex of Photosystem II. Inorganic Chemistry, 2000, 39, 2923-2935.	4.0	154
25	Mechanisms for proton release during water oxidation in the S2 to S3 and S3 to S4 transitions in photosystem II. Physical Chemistry Chemical Physics, 2012, 14, 4849.	2.8	149
26	Modeling the Solvent Sphere:Â Mechanism of the Shilov Reaction. Journal of the American Chemical Society, 1996, 118, 4442-4450.	13.7	145
27	A Density Functional Study of Oâ‚‚ Bond Cleavage for a Biomimetic Non-Heme Iron Complex Demonstrating an FeV-Intermediate. Journal of the American Chemical Society, 2002, 124, 11056-11063.	13.7	145
28	Theoretical Model Studies of the Iron Dimer Complex of MMO and RNR. Inorganic Chemistry, 1999, 38, 2880-2889.	4.0	144
29	Mechanism of Dioxygen Activation in 2-Oxoglutarate-Dependent Enzymes: A Hybrid DFT Study. Chemistry - A European Journal, 2004, 10, 1031-1041.	3.3	144
30	Hydrogen Atom Transfer in Ribonucleotide Reductase (RNR). Journal of Physical Chemistry B, 1998, 102, 10622-10629.	2.6	138
31	Reaction Mechanism of Compound I Formation in Heme Peroxidases:Â A Density Functional Theory Study. Journal of the American Chemical Society, 1999, 121, 10178-10185.	13.7	132
32	Proton Pumping Mechanism in Cytochrome c Oxidase. Journal of Physical Chemistry A, 2008, 112, 12772-12780.	2.5	127
33	A theoretical study of the mechanism for peptide hydrolysis by thermolysin. Journal of Biological Inorganic Chemistry, 2002, 7, 284-298.	2.6	126
34	A Mechanism from Quantum Chemical Studies for Methane Formation in Methanogenesis. Journal of the American Chemical Society, 2002, 124, 4039-4049.	13.7	125
35	Mechanism for Catechol Ring-Cleavage by Non-Heme Iron Extradiol Dioxygenases. Journal of the American Chemical Society, 2004, 126, 8919-8932.	13.7	125
36	A Quantum Chemical Study of Hydrogen Abstraction from Manganese-Coordinated Water by a Tyrosyl Radical:Â A Model for Water Oxidation in Photosystem II. Journal of the American Chemical Society, 1997, 119, 8285-8292.	13.7	124

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37	Oxyl Radical Required for Oâ˜O Bond Formation in Synthetic Mn-Catalyst. Inorganic Chemistry, 2004, 43, 264-274.	4.0	120
38	Modeling Cytochrome Oxidase:Â A Quantum Chemical Study of the Oâ˜O Bond Cleavage Mechanism. Journal of the American Chemical Society, 2000, 122, 12848-12858.	13.7	112
39	Theoretical Study of the Substrate Mechanism of Ribonucleotide Reductase. Journal of the American Chemical Society, 1998, 120, 8417-8429.	13.7	110
40	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. Organometallics, 1997, 16, 1933-1945.	2.3	109
41	Water Oxidation Mechanism for Synthetic Coâ€“Oxides with Small Nuclearity. Journal of the American Chemical Society, 2013, 135, 13804-13813.	13.7	106
42	A theoretical study of the cis-dihydroxylation mechanism in naphthalene 1,2-dioxygenase. Journal of Biological Inorganic Chemistry, 2004, 9, 439-452.	2.6	104
43	Comparisons of results from parametrized configuration interaction (PCIâ€80) and from hybrid density functional theory with experiments for first row transition metal compounds. Journal of Chemical Physics, 1996, 104, 9546-9554.	3.0	103
44	Substrate Water Exchange for the Oxygen Evolving Complex in PSII in the S₁, S₂, and S₃ States. Journal of the American Chemical Society, 2013, 135, 9442-9449.	13.7	102
45	A Quantum Chemical Approach to the Study of Reaction Mechanisms of Redox-Active Metalloenzymes. Journal of Physical Chemistry B, 2001, 105, 9375-9386.	2.6	101
46	Metal-Bridging Mechanism for Oâ˜O Bond Cleavage in Cytochrome c Oxidase. Inorganic Chemistry, 2003, 42, 5231-5243.	4.0	99
47	Nitrogen Fixation by Nitrogenases:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry B, 1998, 102, 1615-1623.	2.6	97
48	A theoretical study on the binding of O2, NO and CO to heme proteins. Journal of Inorganic Biochemistry, 2005, 99, 949-958.	3.5	97
49	Alternative mechanisms for O₂release and Oâ€“O bond formation in the oxygen evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2015, 17, 12168-12174.	2.8	97
50	The Câ€“H activation reaction of methane for all transition metal atoms from the three transition rows. Journal of Chemical Physics, 1997, 107, 4318-4328.	3.0	96
51	An Autocatalytic Mechanism for NiFe-Hydrogenase: Reduction to Ni(I) Followed by Oxidative Addition. Biochemistry, 2009, 48, 1056-1066.	2.5	93
52	Recent theoretical studies of water oxidation in photosystem II. Journal of Photochemistry and Photobiology B: Biology, 2011, 104, 94-99.	3.8	92
53	Model Calculations Suggest that the Central Carbon in the FeMo-Cofactor of Nitrogenase Becomes Protonated in the Process of Nitrogen Fixation. Journal of the American Chemical Society, 2016, 138, 10485-10495.	13.7	92
54	Theoretical Study of the Energetics of Proton Pumping and Oxygen Reduction in Cytochrome Oxidase. Journal of Physical Chemistry B, 2003, 107, 10946-10955.	2.6	90

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55	The Effect of Backbone Constraints: The Case of Water Oxidation by the Oxygenâ€Evolving Complex in PSII. ChemPhysChem, 2011, 12, 3274-3280.	2.1	90
56	4-Hydroxyphenylpyruvate Dioxygenase:â€‰ A Hybrid Density Functional Study of the Catalytic Reaction Mechanism. Biochemistry, 2004, 43, 12331-12342.	2.5	88
57	Theoretical Studies of Oâ‾O Bond Formation in Photosystem II. Inorganic Chemistry, 2008, 47, 1779-1786.	4.0	87
58	Quantum chemical studies of dioxygen activation by mononuclear non-heme iron enzymes with the 2-His-1-carboxylate facial triad. Dalton Transactions, 2004, , 3153.	3.3	84
59	Theoretical investigations of structure and mechanism of the oxygen-evolving complex in PSII. Physical Chemistry Chemical Physics, 2004, 6, 4772.	2.8	84
60	Mechanism for N₂O Generation in Bacterial Nitric Oxide Reductase: A Quantum Chemical Study. Biochemistry, 2012, 51, 5173-5186.	2.5	81
61	Quantum chemical studies of manganese centers in biology. Current Opinion in Chemical Biology, 2002, 6, 227-235.	6.1	80
62	The catalytic cycle of tyrosinase: peroxide attack on the phenolate ring followed by O-O bond cleavage. Journal of Biological Inorganic Chemistry, 2003, 8, 567-576.	2.6	80
63	Reaction Mechanism of Apocarotenoid Oxygenase (ACO): A DFT Study. Chemistry - A European Journal, 2008, 14, 2264-2276.	3.3	79
64	A Density Functional Study on a Biomimetic Non-Heme Iron Catalyst: Insights into Alkane Hydroxylation by a Formally HO?FeV?O Oxidant. Chemistry - A European Journal, 2005, 11, 692-705.	3.3	78
65	An Energetic Comparison of Different Models for the Oxygen Evolving Complex of Photosystem II. Journal of the American Chemical Society, 2009, 131, 18238-18239.	13.7	77
66	On the accuracy of gradient corrected density functional methods for transition metal complexes. Journal of Chemical Physics, 1995, 102, 872-878.	3.0	74
67	Density Functional Calculations of ⁵⁵Mn, ¹⁴N and ¹³C Electron Paramagnetic Resonance Parameters Support an Energetically Feasible Model System for the S₂ State of the Oxygenâ€Evolving Complex of Photosystem II. Chemistry - A European Journal, 2010, 16, 10424-10438.	3.3	73
68	Quantum chemical modeling of CO oxidation by the active site of molybdenum CO dehydrogenase. Journal of Computational Chemistry, 2005, 26, 888-898.	3.3	72
69	Hydrogen transfer in the presence of amino acid radicals. Theoretical Chemistry Accounts, 1997, 97, 289-300.	1.4	71
70	A Quantum Chemical Study of the Mechanism of Tyrosinase. Journal of Physical Chemistry B, 1999, 103, 1193-1202.	2.6	71
71	Activation of Triplet Dioxygen by Glucose Oxidase:â€‰ Spinâ‾Orbit Coupling in the Superoxide Ion. Journal of Physical Chemistry B, 2002, 106, 3742-3750.	2.6	71
72	Catalysis by methyl-coenzyme M reductase: a theoretical study for heterodisulfide product formation. Journal of Biological Inorganic Chemistry, 2003, 8, 653-662.	2.6	70

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73	Mechanism of Aromatic Hydroxylation by an Activated FeIVï£¾O Core in Tetrahydrobiopterin-Dependent Hydroxylases. Chemistry - A European Journal, 2003, 9, 4055-4067.	3.3	69
74	Catalytic Reaction Mechanism of Homogentisate Dioxygenase:Â A Hybrid DFT Study. Journal of the American Chemical Society, 2005, 127, 17303-17314.	13.7	69
75	Energy diagrams and mechanism for proton pumping in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 1143-1156.	1.0	69
76	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. International Journal of Quantum Chemistry, 2000, 76, 714-723.	2.0	68
77	The mechanism for dioxygen formation in PSII studied by quantum chemical methods. Photochemical and Photobiological Sciences, 2005, 4, 1035.	2.9	68
78	First row benchmark tests of the parametrized configuration interaction with parameter X (PCIâ€X) scheme. Journal of Chemical Physics, 1995, 102, 5377-5386.	3.0	66
79	Quantum chemistry applied to the mechanisms of transition metal containing enzymesâ€"Cytochromec oxidase, a particularly challenging case. Journal of Computational Chemistry, 2006, 27, 1373-1384.	3.3	66
80	Reduction of nitric oxide in bacterial nitric oxide reductaseâ€"a theoretical model study. Biochimica Et Biophysica Acta - Bioenergetics, 2006, 1757, 240-252.	1.0	65
81	Electronic Structure Calculations for Molecules Containing Transition Metals. Advances in Chemical Physics, 2007, , 333-387.	0.3	65
82	A theoretical study of myoglobin working as a nitric oxide scavenger. Journal of Biological Inorganic Chemistry, 2004, 9, 923-935.	2.6	64
83	Dinuclear manganese complexes for water oxidation: evaluation of electronic effects and catalytic activity. Physical Chemistry Chemical Physics, 2014, 16, 11950.	2.8	64
84	Nucleophilic water attack is not a possible mechanism for Oâ€“O bond formation in photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4966-4968.	7.1	64
85	Mechanism of Dioxygen Cleavage in Tetrahydrobiopterin-Dependent Amino Acid Hydroxylases. Chemistry - A European Journal, 2003, 9, 106-115.	3.3	63
86	Is the Bis-Î¼-Oxo Cu2(III,III) State an Intermediate in Tyrosinase?. Journal of the American Chemical Society, 2001, 123, 11819-11820.	13.7	61
87	Reaction Mechanism of Water Oxidation Catalyzed by Iron Tetraamido Macrocyclic Ligand Complexes â€“ A DFT Study. European Journal of Inorganic Chemistry, 2014, 2014, 728-741.	2.0	61
88	The S₂ to S₃ transition for water oxidation in PSII (photosystem II), revisited. Physical Chemistry Chemical Physics, 2018, 20, 22926-22931.	2.8	61
89	Quantum Chemical Modeling of Homogeneous Water Oxidation Catalysis. ChemSusChem, 2017, 10, 4236-4263.	6.8	59
90	The mechanism for proton pumping in cytochrome c oxidase from an electrostatic and quantum chemical perspective. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 495-505.	1.0	58

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91	Two, Three, and Four Water Chain Models for the Nucleophilic Addition Step in the Wacker Process. The Journal of Physical Chemistry, 1996, 100, 14672-14680.	2.9	57
92	The mechanism for nitrogenase including all steps. Physical Chemistry Chemical Physics, 2019, 21, 15747-15759.	2.8	57
93	New aspects of H2 activation by nickel-iron hydrogenase. International Journal of Quantum Chemistry, 1999, 73, 197-207.	2.0	56
94	Quantum Chemical Modeling of the Oxidation of Dihydroanthracene by the Biomimetic Nonheme Iron Catalyst [(TMC)Fe^{IV}(O)]²⁺. Journal of Physical Chemistry C, 2007, 111, 12397-12406.	3.1	56
95	Photosystem II Like Water Oxidation Mechanism in a Bioinspired Tetranuclear Manganese Complex. Inorganic Chemistry, 2015, 54, 342-351.	4.0	56
96	The catalytic cycle of catechol oxidase. Journal of Biological Inorganic Chemistry, 2004, 9, 577-590.	2.6	54
97	A theoretical study on nitric oxide reductase activity in a ba3-type heme-copper oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2006, 1757, 31-46.	1.0	53
98	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. Journal of Physical Chemistry A, 1997, 101, 9496-9504.	2.5	51
99	A quantum chemical study of the mechanism of manganese catalase. Theoretical Chemistry Accounts, 2001, 105, 197-206.	1.4	51
100	Catalytic Mechanism of Glyoxalase I:Â A Theoretical Study. Journal of the American Chemical Society, 2001, 123, 10280-10289.	13.7	50
101	Quantum chemical studies of redox-active enzymes. Faraday Discussions, 2003, 124, 289.	3.2	50
102	Quantum chemistry as a tool in bioenergetics. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 129-142.	1.0	50
103	Theoretical study of the reduction of nitric oxide in an A-type flavoprotein. Journal of Biological Inorganic Chemistry, 2006, 12, 79-89.	2.6	49
104	Theoretical studies of enzyme mechanisms involving high-valent iron intermediates. Journal of Inorganic Biochemistry, 2006, 100, 727-743.	3.5	48
105	Energy Diagrams for Water Oxidation in Photosystem II Using Different Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 268-272.	5.3	47
106	A comparison of the thermodynamics of Oâ€“O bond cleavage for dicopper complexes in enzymes and synthetic systems. Journal of Biological Inorganic Chemistry, 2003, 8, 577-585.	2.6	46
107	Water oxidation energy diagrams for photosystem II for different protonation states, and the effect of removing calcium. Physical Chemistry Chemical Physics, 2014, 16, 11893.	2.8	46
108	The mechanism of the Ni-Fe hydrogenases: a quantum chemical perspective. Journal of Biological Inorganic Chemistry, 2001, 6, 460-466.	2.6	45

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109	Exploring pathways and barriers for coupled ET/PT in cytochrome c oxidase: A general framework for examining energetics and mechanistic alternatives. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 244-260.	1.0	45
110	How Is Methane Formed and Oxidized Reversibly When Catalyzed by Niâ€Containing Methylâ€Coenzyme M Reductase?. Chemistry - A European Journal, 2012, 18, 6309-6315.	3.3	45
111	A comparative study of high-spin manganese and iron complexes. Theoretical Chemistry Accounts, 1997, 97, 72-80.	1.4	44
112	A Hybrid Density Functional Study of Oâ^'O Bond Cleavage and Phenyl Ring Hydroxylation for a Biomimetic Non-Heme Iron Complex. Inorganic Chemistry, 2004, 43, 3277-3291.	4.0	44
113	A comparison of the reaction mechanisms of iron- and manganese-containing 2,3-HPCD: an important spin transition for manganese. Journal of Biological Inorganic Chemistry, 2008, 13, 929-940.	2.6	44
114	How Is a Co-Methyl Intermediate Formed in the Reaction of Cobalamin-Dependent Methionine Synthase? Theoretical Evidence for a Two-Step Methyl Cation Transfer Mechanism. Journal of Physical Chemistry B, 2011, 115, 4066-4077.	2.6	44
115	A Systematic DFT Approach for Studying Mechanisms of Redox Active Enzymes. Frontiers in Chemistry, 2018, 6, 644.	3.6	44
116	Mechanism and energy diagram for Oâ€“O bond formation in the oxygen-evolving complex in photosystem II. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1221-1228.	4.0	43
117	Hybrid DFT Study of the Mechanism of Quercetin 2,3-Dioxygenase. Inorganic Chemistry, 2004, 43, 5944-5953.	4.0	41
118	Density Functional Theory Study of the Manganese-Containing Ribonucleotide Reductase from Chlamydia trachomatis: Why Manganese Is Needed in the Active Complex. Biochemistry, 2009, 48, 1878-1887.	2.5	41
119	Role of Substrate Positioning in the Catalytic Reaction of 4-Hydroxyphenylpyruvate Dioxygenaseâ€"A QM/MM Study. Journal of the American Chemical Society, 2014, 136, 14472-14485.	13.7	41
120	Hydroxide instead of bicarbonate in the structure of the oxygen evolving complex. Journal of Inorganic Biochemistry, 2006, 100, 1035-1040.	3.5	40
121	Ethylene Biosynthesis by 1-Aminocyclopropane-1-Carboxylic Acid Oxidase: A DFT Study. Chemistry - A European Journal, 2006, 12, 8835-8846.	3.3	40
122	Mechanism of Water Oxidation Catalyzed by a Mononuclear Manganese Complex. ChemSusChem, 2017, 10, 903-911.	6.8	40
123	Agreement between experiment and hybrid DFT calculations for O?H bond dissociation enthalpies in manganese complexes. Journal of Computational Chemistry, 2005, 26, 661-667.	3.3	39
124	Theoretical Study of the Mechanism of the Nonheme Iron Enzyme EgtB. Inorganic Chemistry, 2017, 56, 3589-3599.	4.0	39
125	Intrinsic Aptitude of Cationic Methyl- and Ethylpalladium To Associate Ethylene and To Further Undergo Subsequent Migratory Insertion. A Theoretical Study. Organometallics, 1996, 15, 5542-5550.	2.3	38
126	Proton pumping in cytochrome c oxidase: Energetic requirements and the role of two proton channels. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1165-1177.	1.0	38

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127	Very Stable Ribonucleotide Substrate Radical Relevant for Class I Ribonucleotide Reductase. Journal of Physical Chemistry B, 2000, 104, 7502-7509.	2.6	37
128	Theoretical study of the catalytic mechanism of catechol oxidase. Journal of Biological Inorganic Chemistry, 2007, 12, 1251-1264.	2.6	37
129	Is There a Ni-Methyl Intermediate in the Mechanism of Methyl-Coenzyme M Reductase?. Journal of the American Chemical Society, 2009, 131, 9912-9913.	13.7	37
130	Harnessing Noninnocent Porphyrin Ligand to Circumvent Fe-Hydride Formation in the Selective Fe-Catalyzed CO₂ Reduction in Aqueous Solution. ACS Catalysis, 2020, 10, 6332-6345.	11.2	37
131	Modeling water exchange on monomeric and dimeric Mn centers. Theoretical Chemistry Accounts, 2003, 110, 130-143.	1.4	35
132	Which Oxidation State Initiates Dehalogenation in the B12-Dependent Enzyme NpRdhA: Co^{II}, Co^I, or Co⁰?. ACS Catalysis, 2015, 5, 7350-7358.	11.2	35
133	A comparison between artificial and natural water oxidation. Dalton Transactions, 2011, 40, 11296.	3.3	34
134	Which Oxidation State Leads to Oâ€“O Bond Formation in Cp*Ir(bpy)Cl-Catalyzed Water Oxidation, Ir(V), Ir(VI), or Ir(VII)?. ACS Catalysis, 2014, 4, 3937-3949.	11.2	34
135	A quantum chemical approach for the mechanisms of redox-active metalloenzymes. RSC Advances, 2021, 11, 3495-3508.	3.6	34
136	A theoretical study of the dioxygen activation by glucose oxidase and copper amine oxidase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2003, 1647, 173-178.	2.3	33
137	Synthesis and Electronâ€Transfer Processes in a New Family of Ligands for Coupled Ruâ^'Mn₂ Complexes. ChemPlusChem, 2014, 79, 936-950.	2.8	33
138	Efficient photochemical water oxidation by a dinuclear molecular ruthenium complex. Chemical Communications, 2015, 51, 1862-1865.	4.1	33
139	A combined picture from theory and experiments on water oxidation, oxygen reduction and proton pumping. Dalton Transactions, 2009, , 5832.	3.3	32
140	Water oxidation in photosystem II: oxygen release, proton release and the effect of chloride. Dalton Transactions, 2009, , 10063.	3.3	32
141	How cytochrome c oxidase can pump four protons per oxygen molecule at high electrochemical gradient. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 364-376.	1.0	32
142	Simulation of the isotropic EXAFS spectra for the S ₂ and S ₃ structures of the oxygen evolving complex in photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3979-3984.	7.1	32
143	The mechanism of hydrogen evolution in Cu(bztpen)-catalysed water reduction: a DFT study. Dalton Transactions, 2015, 44, 9736-9739.	3.3	32
144	A Mechanistic Study of Isopenicillin N Formation Using Density Functional Theory. Journal of the American Chemical Society, 2000, 122, 8539-8547.	13.7	31

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145	Class I ribonucleotide reductase revisited: The effect of removing a proton on Glu441. Journal of Computational Chemistry, 2004, 25, 311-321.	3.3	31
146	Theoretical study of the catalytic reaction mechanism of MndD. Journal of Biological Inorganic Chemistry, 2006, 11, 571-585.	2.6	31
147	Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. International Journal of Quantum Chemistry, 2001, 81, 169-186.	2.0	30
148	Modeling Near-Edge Fine Structure X-ray Spectra of the Manganese Catalytic Site for Water Oxidation in Photosystem II. Journal of the American Chemical Society, 2012, 134, 17157-17167.	13.7	30
149	Important roles of tyrosines in Photosystem II and cytochrome oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2004, 1655, 45-50.	1.0	29
150	Origin of Solvent Acceleration in Organolithium Metalâ^'Halogen Exchange Reactions. Organometallics, 1997, 16, 6021-6023.	2.3	28
151	Quantifying the effects of the self-interaction error in density functional theory: When do the delocalized states appear? II. Iron-oxo complexes and closed-shell substrate molecules. Journal of Chemical Physics, 2008, 129, 154301.	3.0	28
152	An investigation of possible competing mechanisms for Ni-containing methylâ€"coenzyme M reductase. Physical Chemistry Chemical Physics, 2014, 16, 14029.	2.8	28
153	Protonation of the binuclear active site in cytochrome c oxidase decreases the reduction potential of CuB. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1173-1180.	1.0	28
154	Molecular ruthenium water oxidation catalysts carrying non-innocent ligands: mechanistic insight through structureâ€"activity relationships and quantum chemical calculations. Catalysis Science and Technology, 2016, 6, 1306-1319.	4.1	28
155	Is there computational support for an unprotonated carbon in the E₄ state of nitrogenase?. Journal of Computational Chemistry, 2018, 39, 743-747.	3.3	28
156	A Major Structural Change of the Homocitrate Ligand of Probable Importance for the Nitrogenase Mechanism. Inorganic Chemistry, 2018, 57, 1090-1095.	4.0	28
157	A Quantum Chemical Study of the Synthesis of Prostaglandin G2by the Cyclooxygenase Active Site in Prostaglandin Endoperoxide H Synthase 1. Journal of Physical Chemistry B, 2003, 107, 3297-3308.	2.6	27
158	Oxygen Activation by Rieske Non-Heme Iron Oxygenases, a Theoretical Insight. Journal of Physical Chemistry B, 2004, 108, 13031-13041.	2.6	27
159	Catalytic Reaction Mechanism of Oxalate Oxidase (Germin). A Hybrid DFT Study. Journal of Chemical Theory and Computation, 2005, 1, 686-693.	5.3	26
160	Comparison of QM-only and QM/MM models for the mechanism of tyrosinase. Faraday Discussions, 2011, 148, 109-117.	3.2	26
161	Oxygen cleavage with manganese and iron in ribonucleotide reductase from Chlamydia trachomatis. Journal of Biological Inorganic Chemistry, 2011, 16, 553-565.	2.6	26
162	Metal Oxidation States for the Oâ€"O Bond Formation in the Water Oxidation Catalyzed by a Pentanuclear Iron Complex. ACS Catalysis, 2018, 8, 11671-11678.	11.2	26

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163	DFT Study on the Catalytic Reactivity of a Functional Model Complex for Intradiol-Cleaving Dioxygenases. Journal of Physical Chemistry B, 2010, 114, 5878-5885.	2.6	25
164	Why is the reduction of NO in cytochrome c dependent nitric oxide reductase (cNOR) not electrogenic?. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 826-833.	1.0	25
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