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 Mechanism for Nitrogenase Including Loss of a Sulfide. Chemistry - A European Journal, 2022, 28, e202103745.	3.3	20
2	Energetics for CO₂ Reduction by Molybdenum-Containing Formate Dehydrogenase. Journal of Physical Chemistry B, 2022, 126, 1728-1733.	2.6	6
3	The active <scp>E4</scp> structure of nitrogenase studied with different <scp>DFT</scp> functionals. Journal of Computational Chemistry, 2021, 42, 81-85.	3.3	10
4	A quantum chemical approach for the mechanisms of redox-active metalloenzymes. RSC Advances, 2021, 11, 3495-3508.	3.6	34
5	A Theoretical Study of the Recently Suggested Mn^{VII} Mechanism for Oâ€“O Bond Formation in Photosystem II. Journal of Physical Chemistry A, 2020, 124, 8011-8018.	2.5	8
6	Energetics for Proton Reduction in FeFe Hydrogenase. Journal of Physical Chemistry A, 2020, 124, 10540-10549.	2.5	5
7	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
8	Theoretical Study of O₂ Reduction and Water Oxidation in Multicopper Oxidases. Journal of Physical Chemistry A, 2020, 124, 5849-5855.	2.5	8
9	The Energetics of Hydrogen Molecule Oxidation in NiFe-hydrogenase. ACS Catalysis, 2020, 10, 5603-5613.	11.2	16
10	Insights into the Chemical Reactivity in Acetyl-CoA Synthase. Inorganic Chemistry, 2020, 59, 15167-15179.	4.0	11
11	Theoretical Studies of Nickel-Dependent Enzymes. Inorganics, 2019, 7, 95.	2.7	15
12	The mechanism for nitrogenase including all steps. Physical Chemistry Chemical Physics, 2019, 21, 15747-15759.	2.8	57
13	Energetics for the Mechanism of Nickel-Containing Carbon Monoxide Dehydrogenase. Inorganic Chemistry, 2019, 58, 7931-7938.	4.0	18
14	Quantum Chemical Study of the Mechanism of Water Oxidation Catalyzed by a Heterotrinuclear Ru₂Mn Complex. ChemSusChem, 2019, 12, 1101-1110.	6.8	13
15	Mechanism of the Dinuclear Iron EnzymepâEAminobenzoate NâEoxygenase from Density Functional Calculations. ChemCatChem, 2019, 11, 601-613.	3.7	7
16	Theoretical study of the mechanism of the manganese catalase KatB. Journal of Biological Inorganic Chemistry, 2019, 24, 103-115.	2.6	4
17	Reflections on Redox States in Enzymes. , 2019, , 83-90.		0
18	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

#	Article	IF	Citations
19	A Major Structural Change of the Homocitrate Ligand of Probable Importance for the Nitrogenase Mechanism. Inorganic Chemistry, 2018, 57, 1090-1095.	4.0	28
20	A Systematic DFT Approach for Studying Mechanisms of Redox Active Enzymes. Frontiers in Chemistry, 2018, 6, 644.	3.6	44
21	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
22	The S₂ to S₃ transition for water oxidation in PSII (photosystem II), revisited. Physical Chemistry Chemical Physics, 2018, 20, 22926-22931.	2.8	61
23	Metalâ€“Ligand Cooperation in Single-Site Ruthenium Water Oxidation Catalysts: A Combined Experimental and Quantum Chemical Approach. Inorganic Chemistry, 2018, 57, 10881-10895.	4.0	15
24	Theoretical Study of the Mechanism of the Nonheme Iron Enzyme EgtB. Inorganic Chemistry, 2017, 56, 3589-3599.	4.0	39
25	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
26	Mechanism of Water Oxidation Catalyzed by a Mononuclear Manganese Complex. ChemSusChem, 2017, 10, 903-911.	6.8	40
27	Quantum Chemical Modeling of Homogeneous Water Oxidation Catalysis. ChemSusChem, 2017, 10, 4236-4263.	6.8	59
28	Cluster size convergence for the energetics of the oxygen evolving complex in PSII. Journal of Computational Chemistry, 2017, 38, 2157-2160.	3.3	6
29	Chemical and Photochemical Water Oxidation Mediated by an Efficient Singleâ€Site Ruthenium Catalyst. ChemSusChem, 2016, 9, 3448-3456.	6.8	15
30	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
31	Unraveling the Mechanism and Regioselectivity of the B12â€Dependent Reductive Dehalogenase PceA. Chemistry - A European Journal, 2016, 22, 12391-12399.	3.3	25
32	Improved free energy profile for reduction of NO in cytochrome c dependent nitric oxide reductase (cNOR). Journal of Computational Chemistry, 2016, 37, 1810-1818.	3.3	22
33	On the mechanism of water oxidation catalyzed by a dinuclear ruthenium complex: a quantum chemical study. Catalysis Science and Technology, 2016, 6, 5031-5041.	4.1	15
34	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
35	Water Oxidation for Simplified Models of the Oxygenâ€Evolving Complex in Photosystemâ€…II. Chemistry - A European Journal, 2015, 21, 18821-18827.	3.3	11
36	Phosphate Hydrolysis by the Fe₂â€“Ca₃-Dependent Alkaline Phosphatase PhoX: Mechanistic Insights from DFT calculations. Inorganic Chemistry, 2015, 54, 11941-11947.	4.0	3

#	Article	IF	Citations
37	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
38	Electrocatalytic Water Oxidation by a Dinuclear Copper Complex in a Neutral Aqueous Solution. Angewandte Chemie - International Edition, 2015, 54, 4909-4914.	13.8	228
39	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
40	Mechanism and selectivity of the dinuclear iron benzoyl-coenzyme A epoxidase BoxB. Chemical Science, 2015, 6, 2754-2764.	7.4	25
41	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
42	The mechanism of hydrogen evolution in Cu(bztpen)-catalysed water reduction: a DFT study. Dalton Transactions, 2015, 44, 9736-9739.	3.3	32
43	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
44	A Dinuclear Rutheniumâ€Based Water Oxidation Catalyst: Use of Nonâ€Innocent Ligand Frameworks for Promoting Multiâ€Electron Reactions. Chemistry - A European Journal, 2015, 21, 10039-10048.	3.3	22
45	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
46	Mechanism for OO bond formation in a biomimetic tetranuclear manganese cluster â€“ A density functional theory study. Journal of Photochemistry and Photobiology B: Biology, 2015, 152, 162-172.	3.8	20
47	Photosystem II Like Water Oxidation Mechanism in a Bioinspired Tetranuclear Manganese Complex. Inorganic Chemistry, 2015, 54, 342-351.	4.0	56
48	Efficient photochemical water oxidation by a dinuclear molecular ruthenium complex. Chemical Communications, 2015, 51, 1862-1865.	4.1	33
49	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
50	Synthesis and Electronâ€Transfer Processes in a New Family of Ligands for Coupled Ruâ"Mn₂ Complexes. ChemPlusChem, 2014, 79, 936-950.	2.8	33
51	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
52	Quantum Chemical Studies of Mechanisms for Metalloenzymes. Chemical Reviews, 2014, 114, 3601-3658.	47.7	494
53	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
54	Dinuclear manganese complexes for water oxidation: evaluation of electronic effects and catalytic activity. Physical Chemistry Chemical Physics, 2014, 16, 11950.	2.8	64

#	Article	IF	Citations
55	An investigation of possible competing mechanisms for Ni-containing methylâ€“coenzyme M reductase. Physical Chemistry Chemical Physics, 2014, 16, 14029.	2.8	28
56	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
57	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
58	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
59	Mutations in the Dâ€channel of cytochrome c oxidase causes leakage of the proton pump. FEBS Letters, 2014, 588, 545-548.	2.8	10
60	Theoretical Study of the Oxidation of Phenolates by the [Cu₂O₂(N,Nâ€²â€diâ€tertâ€butylethylenediamine)₂]²⁺ Complex. Chemistry - A European Journal, 2013, 19, 1942-1954.	3.8	30
61	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
62	Water Oxidation Mechanism for Synthetic Coâ€“Oxides with Small Nuclearity. Journal of the American Chemical Society, 2013, 135, 13804-13813.	13.7	106
63	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
64	Activation of Dimanganese Class Ib Ribonucleotide Reductase by Hydrogen Peroxide: Mechanistic Insights from Density Functional Theory. Inorganic Chemistry, 2013, 52, 4173-4184.	4.0	7
65	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
66	Nâ€“O bond cleavage mechanism(s) in nitrous oxide reductase. Journal of Biological Inorganic Chemistry, 2012, 17, 687-698.	2.6	24
67	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
68	Mechanism for N₂O Generation in Bacterial Nitric Oxide Reductase: A Quantum Chemical Study. Biochemistry, 2012, 51, 5173-5186.	2.5	81
69	The alkenyl migration mechanism catalyzed by extradiol dioxygenases: a hybrid DFT study. Journal of Biological Inorganic Chemistry, 2012, 17, 881-890.	2.6	12
70	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
71	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
72	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

#	Article	IF	Citations
73	A comparison of two-electron chemistry performed by the manganese and iron heterodimer and homodimers. Journal of Biological Inorganic Chemistry, 2012, 17, 363-373.	2.6	11
74	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
75	Comparison of QM-only and QM/MM models for the mechanism of tyrosinase. Faraday Discussions, 2011, 148, 109-117.	3.2	26
76	A comparison between artificial and natural water oxidation. Dalton Transactions, 2011, 40, 11296.	3.3	34
77	Chapter 13. Theoretical Studies of Oâ€“O and Hâ€“H Bond Formation in Enzymes. RSC Energy and Environment Series, 2011, , 387-407.	0.5	0
78	Oxygen cleavage with manganese and iron in ribonucleotide reductase from Chlamydia trachomatis. Journal of Biological Inorganic Chemistry, 2011, 16, 553-565.	2.6	26
79	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
80	Recent theoretical studies of water oxidation in photosystem II. Journal of Photochemistry and Photobiology B: Biology, 2011, 104, 94-99.	3.8	92
81	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
82	On the observation of a gem diol intermediate after Oâ€“O bond cleavage by extradiol dioxygenases. A hybrid DFT study. Journal of Molecular Modeling, 2010, 16, 1673-1677.	1.8	16
83	Quantum chemistry as a tool in bioenergetics. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 129-142.	1.0	50
84	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
85	Bondâ€dissociation using hybrid DFT. International Journal of Quantum Chemistry, 2010, 110, 317-322.	2.0	11
86	Significant van der Waals Effects in Transition Metal Complexes. Journal of Chemical Theory and Computation, 2010, 6, 2040-2044.	5.3	185
87	Quantum Chemical Studies of Proton-Coupled Electron Transfer in Metalloenzymes. Chemical Reviews, 2010, 110, 7040-7061.	47.7	186
88	Theoretical study of the hydroxylation of phenolates by the Cu2O2(N,Nâ€²-dimethylethylenediamine)2 2+ complex. Journal of Biological Inorganic Chemistry, 2009, 14, 229-242.	2.6	17
89	Theoretical study of the hydroxylation of phenols mediated by an end-on bound superoxoâ€“copper(II) complex. Journal of Biological Inorganic Chemistry, 2009, 14, 273-285.	2.6	12
90	An Autocatalytic Mechanism for NiFe-Hydrogenase: Reduction to Ni(I) Followed by Oxidative Addition. Biochemistry, 2009, 48, 1056-1066.	2.5	93

#	Article	IF	Citations
91	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
92	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
93	A combined picture from theory and experiments on water oxidation, oxygen reduction and proton pumping. Dalton Transactions, 2009, , 5832.	3.3	32
94	Structures and Energetics for O₂ Formation in Photosystem II. Accounts of Chemical Research, 2009, 42, 1871-1880.	15.6	485
95	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
96	Water oxidation in photosystem II: oxygen release, proton release and the effect of chloride. Dalton Transactions, 2009, , 10063.	3.3	32
97	Recent developments of the quantum chemical cluster approach for modeling enzyme reactions. Journal of Biological Inorganic Chemistry, 2009, 14, 643-651.	2.6	257
98	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
99	Reaction Mechanism of Apocarotenoid Oxygenase (ACO): A DFT Study. Chemistry - A European Journal, 2008, 14, 2264-2276.	3.3	79
100	A Structureâ€Consistent Mechanism for Dioxygen Formation in Photosystem II. Chemistry - A European Journal, 2008, 14, 8290-8302.	3.3	215
101	Proton Pumping Mechanism in Cytochrome c Oxidase. Journal of Physical Chemistry A, 2008, 112, 12772-12780.	2.5	127
102	Theoretical Studies of Oâ¯O Bond Formation in Photosystem II. Inorganic Chemistry, 2008, 47, 1779-1786.	4.0	87
103	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
104	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
105	Electronic Structure Calculations for Molecules Containing Transition Metals. Advances in Chemical Physics, 2007, , 333-387.	0.3	65
106	Computational Studies of [NiFe] and [FeFe] Hydrogenases. Chemical Reviews, 2007, 107, 4414-4435.	47.7	383
107	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
108	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

#	Article	IF	Citations
109	Energy diagrams and mechanism for proton pumping in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 1143-1156.	1.0	69
110	Theoretical study of the catalytic mechanism of catechol oxidase. Journal of Biological Inorganic Chemistry, 2007, 12, 1251-1264.	2.6	37
111	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
112	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
113	Density Functional Study of the O2Binding to [CuI(TPAR)]+(TPA = Tris(2-pyridylmethyl)amine) in THF and EtCN. Inorganic Chemistry, 2006, 45, 1491-1497.	4.0	10
114	Modeling Enzymatic Reactions Involving Transition Metals. Accounts of Chemical Research, 2006, 39, 729-738.	15.6	301
115	Theoretical studies of enzyme mechanisms involving high-valent iron intermediates. Journal of Inorganic Biochemistry, 2006, 100, 727-743.	3.5	48
116	Hydroxide instead of bicarbonate in the structure of the oxygen evolving complex. Journal of Inorganic Biochemistry, 2006, 100, 1035-1040.	3.5	40
117	Theoretical study of the catalytic reaction mechanism of MndD. Journal of Biological Inorganic Chemistry, 2006, 11, 571-585.	2.6	31
118	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
119	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
120	Ethylene Biosynthesis by 1-Aminocyclopropane-1-Carboxylic Acid Oxidase: A DFT Study. Chemistry - A European Journal, 2006, 12, 8835-8846.	3.3	40
121	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
122	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
123	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
124	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
125	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
126	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

#	Article	IF	Citations
127	Methods and models for studying mechanisms of redox-active enzymes. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 847-860.	3.4	21
128	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
129	Catalytic Reaction Mechanism of Oxalate Oxidase (Germin). A Hybrid DFT Study. Journal of Chemical Theory and Computation, 2005, 1, 686-693.	5.3	26
130	Catalytic Reaction Mechanism of Homogentisate Dioxygenase:Â A Hybrid DFT Study. Journal of the American Chemical Society, 2005, 127, 17303-17314.	13.7	69
131	Optimized Spin Crossings and Transition States for Short-range Electron Transfer in Transition Metal Dimers. Journal of Physical Chemistry B, 2005, 109, 10513-10520.	2.6	15
132	The mechanism for dioxygen formation in PSII studied by quantum chemical methods. Photochemical and Photobiological Sciences, 2005, 4, 1035.	2.9	68
133	Spin Transition during H2O2Formation in the Oxidative Half-Reaction of Copper Amine Oxidases. Journal of Physical Chemistry B, 2004, 108, 13882-13892.	2.6	24
134	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
135	The catalytic cycle of catechol oxidase. Journal of Biological Inorganic Chemistry, 2004, 9, 577-590.	2.6	54
136	A theoretical study of myoglobin working as a nitric oxide scavenger. Journal of Biological Inorganic Chemistry, 2004, 9, 923-935.	2.6	64
137	Class I ribonucleotide reductase revisited: The effect of removing a proton on Glu441. Journal of Computational Chemistry, 2004, 25, 311-321.	3.3	31
138	Mechanism of Dioxygen Activation in 2-Oxoglutarate-Dependent Enzymes: A Hybrid DFT Study. Chemistry - A European Journal, 2004, 10, 1031-1041.	3.3	144
139	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
140	Theoretical investigations of structure and mechanism of the oxygen-evolving complex in PSII. Physical Chemistry Chemical Physics, 2004, 6, 4772.	2.8	84
141	Oxyl Radical Required for Oâ^'O Bond Formation in Synthetic Mn-Catalyst. Inorganic Chemistry, 2004, 43, 264-274.	4.0	120
142	Hybrid DFT Study of the Mechanism of Quercetin 2,3-Dioxygenase. Inorganic Chemistry, 2004, 43, 5944-5953.	4.0	41
143	4-Hydroxyphenylpyruvate Dioxygenase:â€‰ A Hybrid Density Functional Study of the Catalytic Reaction Mechanism. Biochemistry, 2004, 43, 12331-12342.	2.5	88
144	Oxygen Activation by Rieske Non-Heme Iron Oxygenases, a Theoretical Insight. Journal of Physical Chemistry B, 2004, 108, 13031-13041.	2.6	27

#	Article	IF	Citations
145	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
146	Mechanism for Catechol Ring-Cleavage by Non-Heme Iron Extradiol Dioxygenases. Journal of the American Chemical Society, 2004, 126, 8919-8932.	13.7	125
147	Important roles of tyrosines in Photosystem II and cytochrome oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2004, 1655, 45-50.	1.0	29
148	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
149	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
150	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
151	Modeling water exchange on monomeric and dimeric Mn centers. Theoretical Chemistry Accounts, 2003, 110, 130-143.	1.4	35
152	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
153	A comparison of the mechanism for the reductive half-reaction between pea seedling and other copper amine oxidases (CAOs). Journal of Computational Chemistry, 2003, 24, 1599-1609.	3.3	4
154	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
155	Mechanism of Dioxygen Cleavage in Tetrahydrobiopterin-Dependent Amino Acid Hydroxylases. Chemistry - A European Journal, 2003, 9, 106-115.	3.3	63
156	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
157	Theoretical Study of the Mechanism for the Oxidative Half-Reaction of Copper Amine Oxidase (CAO). Journal of Physical Chemistry B, 2003, 107, 3944-3953.	2.6	18
158	Metal-Bridging Mechanism for Oâ^'O Bond Cleavage in Cytochrome c Oxidase. Inorganic Chemistry, 2003, 42, 5231-5243.	4.0	99
159	Quantum Chemical Studies of Radical-Containing Enzymes. Chemical Reviews, 2003, 103, 2421-2456.	47.7	266
160	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
161	Quantum chemical studies of redox-active enzymes. Faraday Discussions, 2003, 124, 289.	3.2	50
162	A quantum chemical study of tyrosyl reduction and Oâ€"O bond formation in photosystem II. Molecular Physics, 2003, 101, 323-333.	1.7	14

#	Article	IF	Citations
163	Mechanisms of metalloenzymes studied by quantum chemical methods. Quarterly Reviews of Biophysics, 2003, 36, 91-145.	5.7	171
164	Activation of Triplet Dioxygen by Glucose Oxidase:â€‰ Spinâˆ’Orbit Coupling in the Superoxide Ion. Journal of Physical Chemistry B, 2002, 106, 3742-3750.	2.6	71
165	A Mechanism from Quantum Chemical Studies for Methane Formation in Methanogenesis. Journal of the American Chemical Society, 2002, 124, 4039-4049.	13.7	125
166	A Density Functional Study of Oâˆ’O 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
167	A theoretical study of the mechanism for peptide hydrolysis by thermolysin. Journal of Biological Inorganic Chemistry, 2002, 7, 284-298.	2.6	126
168	Quantum chemical studies of manganese centers in biology. Current Opinion in Chemical Biology, 2002, 6, 227-235.	6.1	80
169	A Theoretical Study of the Mechanism for the Reductive Half-Reaction of Pea Seedling Amine Oxidase (PSAO). Journal of Physical Chemistry B, 2001, 105, 4400-4408.	2.6	16
170	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
171	Catalytic Mechanism of Glyoxalase I:Â A Theoretical Study. Journal of the American Chemical Society, 2001, 123, 10280-10289.	13.7	50
172	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
173	A quantum chemical study of the mechanism of manganese catalase. Theoretical Chemistry Accounts, 2001, 105, 197-206.	1.4	51
174	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
175	The mechanism of the Ni-Fe hydrogenases: a quantum chemical perspective. Journal of Biological Inorganic Chemistry, 2001, 6, 460-466.	2.6	45
176	Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. International Journal of Quantum Chemistry, 2001, 81, 169-186.	2.0	1
177	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
178	A density functional theory study of a concerted mechanism for proton exchange between amino acid side chains and water. Theoretical Chemistry Accounts, 2000, 104, 461-470.	1.4	16
179	Modeling Cytochrome Oxidase:Â A Quantum Chemical Study of the Oâˆ’O Bond Cleavage Mechanism. Journal of the American Chemical Society, 2000, 122, 12848-12858.	13.7	112
180	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

#	Article	IF	Citations
181	Transition-Metal Systems in Biochemistry Studied by High-Accuracy Quantum Chemical Methods. Chemical Reviews, 2000, 100, 421-438.	47.7	559
182	Very Stable Ribonucleotide Substrate Radical Relevant for Class I Ribonucleotide Reductase. Journal of Physical Chemistry B, 2000, 104, 7502-7509.	2.6	37
183	A Mechanistic Study of Isopenicillin N Formation Using Density Functional Theory. Journal of the American Chemical Society, 2000, 122, 8539-8547.	13.7	31
184	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. , 2000, 76, 714.		1
185	Ligands with radical character for high oxidation states in manganese and iron complexes. Molecular Physics, 1999, 96, 571-581.	1.7	10
186	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
187	Transition States in Catalysis and Biochemistry. ACS Symposium Series, 1999, , 49-60.	0.5	5
188	New aspects of H2 activation by nickel-iron hydrogenase. International Journal of Quantum Chemistry, 1999, 73, 197-207.	2.0	56
189	DENSITYFUNCTIONALTHEORY OFBIOLOGICALLYRELEVANTMETALCENTERS. Annual Review of Physical Chemistry, 1999, 50, 221-249.	10.8	250
190	A Quantum Chemical Study of the Mechanism of Tyrosinase. Journal of Physical Chemistry B, 1999, 103, 1193-1202.	2.6	71
191	Theoretical Model Studies of the Iron Dimer Complex of MMO and RNR. Inorganic Chemistry, 1999, 38, 2880-2889.	4.0	144
192	The Dehydration Step in the Enzyme-Coenzyme-B12 Catalyzed Diol Dehydrase Reaction of 1,2-Dihydroxyethane Utilizing a Hydrogen-Bonded Carboxylic Acid Group as an Additional Cofactor:â€‰ A Computational Study. Journal of Physical Chemistry B, 1999, 103, 7531-7541.	2.6	18
193	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
194	Hydration of Beryllium, Magnesium, Calcium, and Zinc Ions Using Density Functional Theory. Journal of Physical Chemistry A, 1998, 102, 219-228.	2.5	487
195	Nitrogen Fixation by Nitrogenases:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry B, 1998, 102, 1615-1623.	2.6	97
196	Theoretical Study of the Substrate Mechanism of Ribonucleotide Reductase. Journal of the American Chemical Society, 1998, 120, 8417-8429.	13.7	110
197	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
198	Hydrogen Atom Transfer in Ribonucleotide Reductase (RNR). Journal of Physical Chemistry B, 1998, 102, 10622-10629.	2.6	138

#	Article	IF	Citations
199	Calculating Bond Strengths for Transition-Metal Complexes. ACS Symposium Series, 1998, , 197-211.	0.5	10
200	Mechanism of Hâ^'H Activation by Nickelâ^'Iron Hydrogenase. Journal of the American Chemical Society, 1998, 120, 548-555.	13.7	173
201	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
202	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. Journal of Physical Chemistry A, 1997, 101, 9496-9504.	2.5	51
203	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. Organometallics, 1997, 16, 1933-1945.	2.3	109
204	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
205	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
206	Origin of Solvent Acceleration in Organolithium Metalâ^'Halogen Exchange Reactions. Organometallics, 1997, 16, 6021-6023.	2.3	28
207	A comparative study of high-spin manganese and iron complexes. Theoretical Chemistry Accounts, 1997, 97, 72-80.	1.4	44
208	Hydrogen transfer in the presence of amino acid radicals. Theoretical Chemistry Accounts, 1997, 97, 289-300.	1.4	71
209	Consequences of the Formation of an Organometallic Exciplex [Hg(Î·2-arene)] in Mercury-Photosensitized Reactions of Arenes:Â Câ^'C, Câ^'O, and Câ^'N Bond Cleavage. Organometallics, 1996, 15, 1157-1165.	2.3	8
210	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
211	Modeling the Solvent Sphere:Â Mechanism of the Shilov Reaction. Journal of the American Chemical Society, 1996, 118, 4442-4450.	13.7	145
212	A New Intermolecular Interaction:â€‰ UnconventionalHydrogen Bonds with Elementâ^'Hydride Bonds as ProtonAcceptor. Accounts of Chemical Research, 1996, 29, 348-354.	15.6	639
213	Models for the description of the H3O+ and OH? ions in water. Journal of Computational Chemistry, 1996, 17, 1099-1107.	3.3	11
214	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
215	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
216	On the accuracy of gradient corrected density functional methods for transition metal complexes. Journal of Chemical Physics, 1995, 102, 872-878.	3.0	74

#	Article	IF	Citations
217	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
218	Oxygen chemisorption on metal surfaces using the cluster model: Basis set effects. Theoretica Chimica Acta, 1991, 79, 413-418.	0.8	4