Kizashi Yamaguchi

List of Publications by Year
in descending order

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433	12,834	39113	43601
papers	citations	52 h-index	95 g-index

433	433	433	6662
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relative energies among proton-shifted S2 isomers in the photosystem II revealed by DLPNO coupled cluster and hybrid DFT calculations. Proton transfer coupled spin transitions of the CaMn4Ox cluster in OEC of PSII. Chemical Physics Letters, 2022, 790, 139357.	1.2	5
2	Relative energies among S3 intermediates in the photosystem II revealed by DLPNO coupled cluster and hybrid DFT calculations. Possible pathways of water insertion in the S2 to S3 transition. Chemical Physics Letters, 2022, 793, 139439.	1.2	8
3	A three states model for hydrogen abstraction reactions with the cytochrome P450 compound I is revisited. Isolobal and isospin analogy among Fe(IV)=O, Oâ€¯=â€¯O and O. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 405, 112902.	2.0	3
4	Relative stability among intermediate structures in S2 state of CaMn4O5 cluster in PSII by using hybrid-DFT and DLPNO-CC methods and evaluation of magnetic interactions between Mn ions. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 405, 112923.	2.0	7
5	Mechanism of Water Oxidation in Photosynthesis Elucidated by Interplay Between Experiment and Theory. Advances in Photosynthesis and Respiration, 2021, , 39-80.	1.0	0
6	Estimation of spin contamination errors in DFT/plane-wave calculations of solid materials using approximate spin projection scheme. Chemical Physics Letters, 2021, 765, 138291.	1.2	14
7	Isolobal and isospin analogy between organic and inorganic open-shell moleculesâ€”Application to oxygenation reactions by active oxygen and oxy-radicals and water oxidation in the native and artificial photosynthesis. Advances in Quantum Chemistry, 2021, , 425-564.	0.4	1
8	Domain-based local pair natural orbital CCSD(T) calculations of strongly correlated electron systems: Examination of dynamic equilibrium models based on multiple intermediates in S₁ state of photosystem II. Molecular Physics, 2020, 118, e1666171.	0.8	3
9	Comparison of Effective Exchange Integrals of H-H and H-He-H Chains vs. Single Molecules: A Theoretical Study. Chemistry Letters, 2020, 49, 137-140.	0.7	6
10	Development of broken-symmetry (BS) methods in chemical reactions. A theoretical view of water oxidation in photosystem II and related systems. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 402, 112791.	2.0	3
11	Clarification of the Relationship between the Magnetic and Conductive Properties of Infinite Chains in Trioxotriangulene Radical Crystals by Spinâ€Projected DFT/Planeâ€Wave Calculations. Advanced Theory and Simulations, 2020, 3, 2000050.	1.3	10
12	UNO(ULO) active space for multireference calculations on classical and quantum computers. Revisit to the iron-sulfur complexes. Chemical Physics Letters, 2020, 746, 137252.	1.2	2
13	Theory of chemical bonds in metalloenzymes XXIII fundamental principles for the photo-induced water oxidation in oxygen evolving complex of photosystem II. Molecular Physics, 2020, 118, e1725168.	0.8	2
14	Electronic and spin structures of CaMn4Ox clusters in the S0 state of the oxygen evolving complex of photosystem II. Domain-based local pair natural orbital (DLPNO) coupled-cluster (CC) calculations using optimized geometries and natural orbitals (UNO) by hybrid density functional theory (HDFT) calculations. Physical Chemistry Chemical Physics, 2020, 22, 27191-27205.	1.3	5
15	Theory of chemical bonds in metalloenzymes XXIV electronic and spin structures of FeMoco and Fe-S clusters by classical and quantum computing. Molecular Physics, 2020, 118, e1760388.	0.8	5
16	An oxyl/oxo mechanism for oxygen-oxygen coupling in PSII revealed by an x-ray free-electron laser. Science, 2019, 366, 334-338.	6.0	248
17	Domain-based local pair natural orbital CCSD(T) calculations of fourteen different S2 intermediates for water oxidation in the Kok cycle of OEC of PSII. Re-visit to one LS-two HS model for the S2 state. Chemical Physics Letters, 2019, 734, 136731.	1.2	11
18	Spin contamination errors on spin-polarized density functional theory/plane-wave calculations for crystals of one-dimensional materials. Applied Physics Express, 2019, 12, 115506.	1.1	31

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19	Possibility of the right-opened Mn-oxo intermediate (R-oxo(4444)) among all nine intermediates in the S3 state of the oxygen-evolving complex of photosystem II revealed by large-scale QM/MM calculations. Chemical Physics, 2019, 518, 81-90.	0.9	10
20	Domain-based local pair natural orbital CCSD(T) calculations of six different S1 structures of oxygen evolving complex of photosystem II. Proposal of multi-intermediate models for the S1 state. Chemical Physics Letters, 2019, 732, 136660.	1.2	13
21	Elucidation of the entire Kok cycle for photosynthetic water oxidation by the large-scale quantum mechanics/molecular mechanics calculations: Comparison with the experimental results by the recent serial femtosecond crystallography. Chemical Physics Letters, 2019, 730, 416-425.	1.2	8
22	Spin, Valence, and Structural Isomerism in the S₃ State of the Oxygen-Evolving Complex of Photosystem II as a Manifestation of Multimetallic Cooperativity. Journal of Chemical Theory and Computation, 2019, 15, 2375-2391.	2.3	40
23	Linear Response Functions of Densities and Spin Densities for Systematic Modeling of the QM/MM Approach for Mono- and Poly-Nuclear Transition Metal Systems. Molecules, 2019, 24, 821.	1.7	3
24	Theoretical and computational investigations of geometrical, electronic and spin structures of the CaMn 4 O X (Xâ€‰=â€‰5, 6) cluster in the Kok cycle S i (iâ€‰=â€‰0â€“3) of oxygen evolving complex of photosystem II. Physiologia Plantarum, 2019, 166, 44-59.	2.8	14
25	UNO DMRG CAS CI calculations of binuclear manganese complex Mn(IV) 2 O 2 (NHCHCO 2) 4 : Scope and applicability of Heisenberg model. Journal of Computational Chemistry, 2019, 40, 333-341.	1.5	16
26	Theory of chemical bonds in metalloenzymes XXII: a concerted bond-switching mechanism for the oxygenâ€“oxygen bond formation coupled with one electron transfer for water oxidation in the oxygen-evolving complex of photosystem II. Molecular Physics, 2019, 117, 2320-2354.	0.8	7
27	Concerted bond switching mechanism coupled with one-electron transfer for the oxygen-oxygen bond formation in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2019, 714, 219-226.	1.2	17
28	Theoretical Elucidation of Geometrical Structures of the CaMn4O5 Cluster in Oxygen Evolving Complex of Photosystem II Scope and Applicability of Estimation Formulae of Structural Deformations via the Mixed-Valence and Jahnâ€“Teller Effects. Advances in Quantum Chemistry, 2019, , 307-451.	0.4	13
29	Theory of chemical bonds in metalloenzymes XXI. Possible mechanisms of water oxidation in oxygen evolving complex of photosystem II. Molecular Physics, 2018, 116, 717-745.	0.8	33
30	Nonadiabatic one-electron transfer mechanism for the Oâ€“O bond formation in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2018, 698, 138-146.	1.2	28
31	Understanding Two Different Structures in the Dark Stable State of the Oxygenâ€Evolving Complex of Photosystemâ€…II: Applicability of the Jahnâ€“Teller Deformation Formula. ChemPhotoChem, 2018, 2, 257-270.	1.5	9
32	Development of approximate spin projection method and its application for elucidation of electronic structures, molecular structures and physical properties of polynuclear metal complexes. Bulletin of Japan Society of Coordination Chemistry, 2018, 71, 57-68.	0.1	0
33	Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in PhotosystemÂII. Journal of Physical Chemistry B, 2018, 122, 6491-6502.	1.2	21
34	Relative stability between the manganese hydroxide- and oxo-models for water oxidation by CCSD, DMRG CASCI, CASSCF, CASPT2 and CASDFT methods; Importance of static and dynamical electron correlation effects for OEC of PSII. Chemical Physics Letters, 2018, 705, 85-91.	1.2	10
35	The Reaction Mechanisms of O₂ Formation in Photosynthesis. Seibutsu Butsuri, 2018, 58, 127-133.	0.0	0
36	On the guiding principles for understanding of geometrical structures of the CaMn₄O₅cluster in oxygen-evolving complex of photosystem II. Proposal of estimation formula of structural deformations via the Jahnâ€“Teller effects. Molecular Physics, 2017, 115, 636-666.	0.8	16

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37	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. Molecular Physics, 2017, 115, 2154-2167.	0.8	2
38	Large-scale QM/MM calculations of the CaMn₄O₅ cluster in the S₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. Faraday Discussions, 2017, 198, 83-106.	1.6	31
39	Large-scale QM/MM calculations of the CaMn4O5 cluster in the oxygen-evolving complex of photosystem II: Comparisons with EXAFS structures. Chemical Physics Letters, 2016, 658, 354-363.	1.2	15
40	Theoretical Studies on the Magnetic and Conductive Properties of Crystals Containing Open-Shell Trioxotriangulene Radicals. Bulletin of the Chemical Society of Japan, 2016, 89, 315-333.	2.0	15
41	Geometric and electronic structures of the synthetic Mn₄CaO₄ model compound mimicking the photosynthetic oxygen-evolving complex. Physical Chemistry Chemical Physics, 2016, 18, 11330-11340.	1.3	25
42	Chemical Equilibrium Models for the S₃ State of the Oxygen-Evolving Complex of Photosystem II. Inorganic Chemistry, 2016, 55, 502-511.	1.9	90
43	Theory of chemical bonds in metalloenzymes XX: magneto-structural correlations in the CaMn4O5cluster in oxygen-evolving complex of photosystem II. Molecular Physics, 2015, , 1-28.	0.8	7
44	Theoretical Study of Electronic Properties of Phenalenyl Radical and Zethrene Diradical Species: Possibility of Triplet Oxygen Adsorption onto Graphene Surface. Bulletin of the Chemical Society of Japan, 2015, 88, 149-161.	2.0	8
45	First principle calculations of effective exchange integrals: Comparison between SR (BS) and MR computational results. , 2015, , .		0
46	Theoretical studies of the damage-free S1 structure of the CaMn4O5 cluster in oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2015, 623, 1-7.	1.2	29
47	Theoretical modelling of biomolecular systems I. Large-scale QM/MM calculations of hydrogen-bonding networks of the oxygen evolving complex of photosystem II. Molecular Physics, 2015, 113, 359-384.	0.8	28
48	QM/MM study of the S2 to S3 transition reaction in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2015, 636, 172-179.	1.2	79
49	Large-Scale QM/MM Calculations of Hydrogen Bonding Networks for Proton Transfer and Water Inlet Channels for Water Oxidationâ€"Theoretical System Models of the Oxygen-Evolving Complex of Photosystem II. Advances in Quantum Chemistry, 2015, 70, 325-413.	0.4	23
50	On the guiding principles for lucid understanding of the damage-free S1 structure of the CaMn4O5 cluster in the oxygen evolving complex of photosystem II. Chemical Physics Letters, 2015, 627, 44-52.	1.2	26
51	Full geometry optimizations of the CaMn4O4 model cluster for the oxygen evolving complex of photosystem II. Chemical Physics Letters, 2015, 640, 23-30.	1.2	15
52	Strong Coupling between the Hydrogen Bonding Environment and Redox Chemistry during the S₂ to S₃ Transition in the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2015, 119, 13922-13933.	1.2	51
53	Theoretical Investigation on Nearsightedness of Finite Model and Molecular Systems Based on Linear Response Function Analysis. Molecules, 2014, 19, 13358-13373.	1.7	7
54	Generalized approximate spin projection calculations of effective exchange integrals of the CaMn4O5 cluster in the S1 and S3 states of the oxygen evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11911-11923.	1.3	48

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55	Water Oxidation Chemistry of a Synthetic Dinuclear Ruthenium Complex Containing Redox-Active Quinone Ligands. Inorganic Chemistry, 2014, 53, 3973-3984.	1.9	38
56	Theory of chemical bonds in metalloenzymes XIX: labile manganese oxygen bonds of the CaMn₄O₅cluster in oxygen evolving complex of photosystem II. Molecular Physics, 2014, 112, 485-507.	0.8	18
57	An efficient initial guess formation of broken-symmetry solutions by using localized natural orbitals. Chemical Physics Letters, 2014, 608, 50-54.	1.2	17
58	Linear response function approach for the boundary problem of QM/MM methods. International Journal of Quantum Chemistry, 2013, 113, 336-341.	1.0	8
59	Full geometry optimizations of the mixedâ€valence CaMn₄O₄X(H₂O)₄ (X=OH or O) cluster in OEC of PS II: Degree of symmetry breaking of the labile Mnâ€Xâ€Mn bond revealed by several hybrid DFT calculations. International Journal of Quantum Chemistry, 2013, 113, 525-541.	1.0	60
60	The nature of chemical bonds of the CaMn₄O₅ cluster in oxygen evolving complex of photosystem II: Jahnâ€Teller distortion and its suppression by Ca doping in cubane structures. International Journal of Quantum Chemistry, 2013, 113, 453-473.	1.0	60
61	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional Nin (n = 3, 5, 7) complexes. Dalton Transactions, 2013, 42, 16200.	1.6	18
62	Theory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn5O5, CaMn4O5 and Ca2Mn3O5 clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesis. Polyhedron, 2013, 57, 138-149.	1.0	8
63	Reprint of â€œTheory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn5O5, CaMn4O5 and Ca2Mn3O5 clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesisâ€. Polyhedron, 2013, 66, 283-293.	1.0	0
64	Theory of chemical bonds in metalloenzymes XVI. Oxygen activation by high-valent transition metal ions in native and artificial systems. Polyhedron, 2013, 66, 228-244.	1.0	7
65	Electronic Structure of the CaMn4O5 Cluster in the PSII System Refined to the 1.9 Ã... X-ray Resolution. Possible Mechanisms of Photosynthetic Water Splitting. Advanced Topics in Science and Technology in China, 2013, , 250-254.	0.0	0
66	Theoretical insight in to hydrogen-bonding networks and proton wire for the CaMn4O5 cluster of photosystem II. Elongation of Mnâ€“Mn distances with hydrogen bonds. Catalysis Science and Technology, 2013, 3, 1831.	2.1	49
67	Locality and nonlocality of electronic structures of molecular systems: Toward QM/MM and QM/QM approaches. AIP Conference Proceedings, 2012, , .	0.3	6
68	Theory of chemical bonds in metalloenzymes - Manganese oxides clusters in the oxygen evolution center -. AIP Conference Proceedings, 2012, , .	0.3	8
69	Effectiveness of Optimizing Geometry for CaMn4O5 Cluster at 1.9 Ã... Resolved OEC and Proposal for Oxidation Mechanism from S0 to S3 States. Chemistry Letters, 2012, 41, 18-20.	0.7	13
70	Role of Perferrylâ€“Oxo Oxidant in Alkane Hydroxylation Catalyzed by Cytochrome P450: A Hybrid Density Functional Study. Journal of Physical Chemistry B, 2012, 116, 4713-4730.	1.2	22
71	Theoretical illumination of water-inserted structures of the CaMn4O5 cluster in the S2 and S3 states of oxygen-evolving complex of photosystem II: full geometry optimizations by B3LYP hybrid density functional. Dalton Transactions, 2012, 41, 13727.	1.6	176
72	Electronic and Spin Structures of the CaMn4O5(H2O)4 Cluster in OEC of PSII Refined to 1.9Ã... X-ray Resolution. Advances in Quantum Chemistry, 2012, 64, 121-187.	0.4	32

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73	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn₄O₅ cluster of PSII refined to 1.9 Ã... Xâ€ray resolution. International Journal of Quantum Chemistry, 2012, 112, 253-276.	1.0	66
74	Theory of chemical bonds in metalloenzymes. XVII. Symmetry breaking in manganese cluster structures and chameleonic mechanisms for the Oï£¿O bond formation of water splitting reaction. International Journal of Quantum Chemistry, 2012, 112, 121-135.	1.0	21
75	Structure and reactivity of the mixedâ€valence CaMn₄O₅(H₂O)₄ and CaMn₄O₄(OH)(H₂O)₄ clusters at oxygen evolution complex of photosystem II. Hybrid DFT (UB3LYP and UBHandHLYP) calculations. International Journal of Quantum Chemistry, 2012, 112, 321-342.	1.0	48
76	Spin hamiltonian models for artificial and native water splitting systems revealed by hybrid DFT calculations. Oxygen activation by highâ€valent Mn and Ru ions. International Journal of Quantum Chemistry, 2012, 112, 3849-3866.	1.0	20
77	Similarities of artificial photosystems by ruthenium oxo complexes and native water splitting systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15600-15605.	3.3	50
78	Does B3LYP correctly describe magnetism of manganese complexes with various oxidation numbers and various structural motifs?. Chemical Physics Letters, 2012, 519-520, 134-140.	1.2	9
79	Approximate Spin Projection for Geometry Optimization of Biradical Systems: Case Studies of Through-Space and Through-Bond Systems. Progress in Theoretical Chemistry and Physics, 2012, , 345-359.	0.2	1
80	Potential Energy Curve for Ring-Opening Reactions: Comparison Between Broken-Symmetry and Multireference Coupled Cluster Methods. Journal of Physical Chemistry A, 2011, 115, 5625-5631.	1.1	17
81	Theoretical studies on the structural and magnetic property of arginase active site. Supramolecular Chemistry, 2011, 23, 22-28.	1.5	3
82	Theoretical study of absorption spectrum of dirhodium tetracarboxylate complex [Rh2(CH3COO)4(H2O)2] in aqueous solution revisited. Supramolecular Chemistry, 2011, 23, 329-336.	1.5	7
83	Unique Structural and Electronic Features of Perferrylâ€“Oxo Oxidant in Cytochrome P450. Journal of Physical Chemistry B, 2011, 115, 10730-10738.	1.2	23
84	Modification of MOF catalysts by manipulation of counter-ions: experimental and theoretical studies of photochemical hydrogen production from water over microporous diruthenium (II, III) coordination polymers. Supramolecular Chemistry, 2011, 23, 287-296.	1.5	32
85	Theoretical study of intra- and inter-chain magnetic interactions in [Ni(chxn)2Br]Br2. Polyhedron, 2011, 30, 3116-3120.	1.0	8
86	Ab initio study of magnetic interactions of manganese-oxide clusters. Polyhedron, 2011, 30, 3256-3261.	1.0	18
87	Singletâ€“triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. Theoretical Chemistry Accounts, 2011, 130, 739-748.	0.5	30
88	Symmetry and broken symmetry in molecular orbital description of unstable molecules IV: comparison between single- and multi-reference computational results for antiaromtic molecules. Theoretical Chemistry Accounts, 2011, 130, 749-763.	0.5	40
89	Labile electronic and spin states of the CaMn4O5 cluster in the PSII system refined to the 1.9 Ã... X-ray resolution. UB3LYP computational results. Chemical Physics Letters, 2011, 506, 98-103.	1.2	66
90	Broken-symmetry natural orbital (BSNO)â€“Mk-MRCC study on the exchange coupling in the binuclear copper(II) compounds. Chemical Physics Letters, 2011, 505, 11-15.	1.2	20

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91	Possible mechanisms for the Oâ€“O bond formation in oxygen evolution reaction at the CaMn4O5(H2O)4 cluster of PSII refined to 1.9 Ã... X-ray resolution. Chemical Physics Letters, 2011, 511, 138-145.	1.2	96
92	Theoretical studies on the electronic structure of the synthetic complex of soluble methanemonooxygenase intermediate Q. Supramolecular Chemistry, 2011, 23, 83-87.	1.5	2
93	Theoretical Study on the Electronic Configurations and Nature of Chemical Bonds of Dirhodium Tetraacetato Complexes [Rh2(CH3COO)4(L)2] (L = H2O, Free): Broken Symmetry Approach. Bulletin of the Chemical Society of Japan, 2010, 83, 1481-1488.	2.0	11
94	UNOâ€•and ULOâ€•MRCC(Mk), APâ€•UCC and APâ€•UBD approaches to diradical systems. International Journal of Quantum Chemistry, 2010, 110, 3015-3026.	1.0	15
95	Theory of chemical bonds in metalloenzymes. XV. Local singlet and triplet diradical mechanisms for radical coupling reactions in the oxygen evolution complex. International Journal of Quantum Chemistry, 2010, 110, 3101-3128.	1.0	49
96	Theory of chemical bonds in metalloenzymes. XIV. Correspondence between magnetic coupling mode and radical coupling mechanism in hydroxylations with methane monooxygenase and related species. International Journal of Quantum Chemistry, 2010, 110, 2955-2981.	1.0	15
97	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. Molecular Physics, 2010, 108, 2533-2541.	0.8	10
98	MkMRCC, APUCC and APUBD approaches to 1,n-didehydropolyene diradicals: the nature of through-bond exchange interactions. Molecular Physics, 2010, 108, 2559-2578.	0.8	11
99	Instability In Chemical Bonds: Uno Cascc, Resonating Ucc And Approximately Projected Ucc Methods To Quasi-Degenerate Electronic Systems. Challenges and Advances in Computational Chemistry and Physics, 2010, , 621-648.	0.6	1
100	Instability in Chemical Bonds from Broken-Symmetry Single-Reference to Symmetry-Adapted Multireference Approaches to Strongly Correlated Electron Systems. , 2009, , .		9
101	Theory of chemical bonds in metalloenzymes XIII: Singlet and triplet diradical mechanisms of hydroxylations with ironâ€•oxo species and P450 are revisited. International Journal of Quantum Chemistry, 2009, 109, 3723-3744.	1.0	12
102	Estimation of effective exchange integral value of polyradical systems based on the band calculation. International Journal of Quantum Chemistry, 2009, 109, 3632-3640.	1.0	5
103	Extended Hartreeâ€“Fock theory of chemical reactions. IX. Diradical and perepoxide mechanisms for oxygenations of ethylene with molecular oxygen and ironâ€•oxo species are revisited. International Journal of Quantum Chemistry, 2009, 109, 3745-3766.	1.0	12
104	Approximately spinâ€•projected Hessian for broken symmetry method and stretching frequencies of F₂ and singlet O₂. International Journal of Quantum Chemistry, 2009, 109, 3641-3648.	1.0	11
105	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. International Journal of Quantum Chemistry, 2009, 109, 3649-3658.	1.0	10
106	Resonating coupledâ€•cluster CI approach to ionâ€•radical systems: Comparison with the unrestricted coupledâ€•cluster approach. International Journal of Quantum Chemistry, 2009, 109, 3811-3818.	1.0	7
107	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. Polyhedron, 2009, 28, 1945-1949.	1.0	12
108	Theoretical study of magnetic interaction between C60 anion radicals. Polyhedron, 2009, 28, 1750-1753.	1.0	3

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109	Theory of chemical bonds in metalloenzymes XII: Electronic and spin structures of metalloâ€“oxo and isoelectronic species and spin crossover phenomena in oxygenation reactions. Polyhedron, 2009, 28, 2044-2052.	1.0	8
110	Hybrid-DFT Study on Electronic Structures of the Active Site of Sweet Potato Purple Acid Phosphatase: The Origin of Stronger Antiferromagnetic Couplings than Other Purple Acid Phosphatases. Journal of Physical Chemistry A, 2009, 113, 5099-5104.	1.1	8
111	A resonating broken symmetry configuration interaction approach for double-exchange magnetic systems. Journal of Physics Condensed Matter, 2009, 21, 064227.	0.7	8
112	Symmetry and Broken-Symmetry in Molecular Orbital Descriptions of Unstable Molecules. 3. The Nature of Chemical Bonds of Spin Frustrated Systems. Journal of Physical Chemistry A, 2009, 113, 15281-15297.	1.1	11
113	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A1) by Broken-Symmetry Method. Journal of Physical Chemistry A, 2009, 113, 15041-15046.	1.1	68
114	Theory of chemical bonds in metalloenzymes. VII. Hybridâ€density functional theory studies on the electronic structures of P450. International Journal of Quantum Chemistry, 2008, 108, 631-650.	1.0	20
115	Nâ€bands Hubbard models. IV. Comparisons of electronâ€or holeâ€doped quaternary oxypictides LaOMPn superconductors with cuprates. International Journal of Quantum Chemistry, 2008, 108, 3016-3041.	1.0	0
116	Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Feâ€4S clusters. International Journal of Quantum Chemistry, 2008, 108, 2881-2887.	1.0	24
117	Theory of chemical bonds in metalloenzymes XI: Full geometry optimization and vibration analysis of porphyrin ironâ€oxo species. International Journal of Quantum Chemistry, 2008, 108, 2950-2965.	1.0	6
118	Extended Hartreeâ€“Fock theory of chemical reactions. VIII. Hydroxylation reactions by P450. International Journal of Quantum Chemistry, 2008, 108, 2991-3009.	1.0	14
119	CHARGE-TRANSFER-INDUCED LUMINESCENCE (CTIL) MECHANISMS OF CHEMI- AND BIOLUMINESCENCE REACTIONS. , 2008, , .		0
120	THEORETICAL CONSIDERATIONS ON THE ROLES OF HYDROGEN BONDING IN THERMAL DECOMPOSITION OF PEROXIDES. , 2008, , .		0
121	Structure and function of a hexameric copper-containing nitrite reductase. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4315-4320.	3.3	69
122	Derivation of dynamic electric and magnetic response properties based on the quasienergy derivative method. Journal of Computational Methods in Sciences and Engineering, 2007, 6, 397-427.	0.1	0
123	Approximately spin-projected geometry optimization method and its application to di-chromium systems. Chemical Physics Letters, 2007, 442, 445-450.	1.2	129
124	Theoretical studies on relation among structures, electric structures and magnetic interactions in MMX complexes. Polyhedron, 2007, 26, 2154-2160.	1.0	9
125	Theory of chemical bonds in metalloenzymes VI: Manganeseâ€“oxo bonds in the photosynthesis II system. Polyhedron, 2007, 26, 2216-2224.	1.0	48
126	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Feâ€“2S] cluster. International Journal of Quantum Chemistry, 2007, 107, 116-133.	1.0	33

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127	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Feï£¿2S] clusters. International Journal of Quantum Chemistry, 2007, 107, 609-627.	1.0	32
128	Ab initio calculation of the Dzyaloshinskiiâ€“Moriya parameters: Spinâ€“orbit GSO-HF, DFT, and CI approaches. International Journal of Quantum Chemistry, 2007, 107, 1328-1334.	1.0	16
129	Density functional study of manganese dimer. International Journal of Quantum Chemistry, 2007, 107, 3178-3190.	1.0	21
130	Geometry optimization method based on approximate spin projection and its application to F₂, CH₂, CH₂OO, and active site of urease. International Journal of Quantum Chemistry, 2007, 107, 3094-3102.	1.0	24
131	Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase and the related species. International Journal of Quantum Chemistry, 2007, 107, 3250-3265.	1.0	13
132	Spinâ€optimized resonating Hartreeâ€Fock configuration interaction. International Journal of Quantum Chemistry, 2007, 107, 3219-3227.	1.0	5
133	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. Molecular Crystals and Liquid Crystals, 2006, 455, 135-141.	0.4	1
134	Recent Development of Multireference Density Functional Theory. Chemistry Letters, 2006, 35, 242-247.	0.7	25
135	The Nature of Effective Exchange Interactions. , 2006, , 201-228.		3
136	N-band Hubbard models. III. Boson-fermion and interaction-boson models for high-Tcsuperconductivity. International Journal of Quantum Chemistry, 2006, 106, 1052-1075.	1.0	4
137	CASSCF version of density functional theory. International Journal of Quantum Chemistry, 2006, 106, 3325-3333.	1.0	18
138	Multireference density functional theory with orbital-dependent correlation corrections. International Journal of Quantum Chemistry, 2006, 106, 3312-3324.	1.0	33
139	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Feâ€“7S] core. International Journal of Quantum Chemistry, 2006, 106, 3288-3302.	1.0	28
140	Resonating broken-symmetry approach to biradicals and polyradicals. International Journal of Quantum Chemistry, 2006, 106, 3303-3311.	1.0	20
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