Kizashi Yamaguchi

List of Publications by Year
in descending order

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433 papers	12,834 citations	34105 52 h-index	38395 95 g-index
433 all docs	433 docs citations	433 times ranked	5952 citing authors

#	Article	IF	Citations
1	A spin correction procedure for unrestricted Hartree-Fock and MÃ¸ller-Plesset wavefunctions for singlet diradicals and polyradicals. Chemical Physics Letters, 1988, 149, 537-542.	2.6	720
2	Ab initio computations of effective exchange integrals for Hâ€“H, Hâ€“Heâ€“H and Mn2O2 complex: comparison of broken-symmetry approaches. Chemical Physics Letters, 2000, 319, 223-230.	2.6	675
3	The electronic structures of biradicals in the unrestricted Hartree-Fock approximation. Chemical Physics Letters, 1975, 33, 330-335.	2.6	384
4	Mapping of the Hot Spots for DNA Damage by One-Electron Oxidation: Efficacy of GG Doublets and GGG Triplets as a Trap in Long-Range Hole Migration. Journal of the American Chemical Society, 1998, 120, 12686-12687.	13.7	352
5	Effective exchange integrals for open-shell species by density functional methods. Chemical Physics Letters, 1994, 231, 25-33.	2.6	304
6	Distribution of odd electrons in ground-state molecules. Theoretica Chimica Acta, 1978, 48, 175-183.	0.8	292
7	Ab-Initio Molecular Orbital Studies of Structure and Reactivity of Transition Metal-OXO Compounds. , 1986, , 155-184.		283
8	A general algorithm for calculation of Heisenberg exchange integrals J in multispin systems. Chemical Physics Letters, 2006, 432, 343-347.	2.6	268
9	Sizeâ€consistent approach and density analysis of hyperpolarizability: Second hyperpolarizabilities of polymeric systems with and without defects. Journal of Chemical Physics, 1995, 103, 4175-4191.	3.0	250
10	An oxyl/oxo mechanism for oxygen-oxygen coupling in PSII revealed by an x-ray free-electron laser. Science, 2019, 366, 334-338.	12.6	248
11	Extended Hartree-Fock (EHF) theory of chemical reactions. Theoretica Chimica Acta, 1988, 73, 337-364.	0.8	214
12	Ab Initio MO Calculations of Effective Exchange Integrals between Transition-Metal Ions via Oxygen Dianions: Nature of the Copper-Oxygen Bonds and Superconductivity. Japanese Journal of Applied Physics, 1987, 26, L1362-L1364.	1.5	207
13	MOLECULAR ORBITAL (MO) THEORY FOR MAGNETICALLY INTERACTING ORGANIC COMPOUNDS. AB-INITIO MO CALCULATIONS OF THE EFFECTIVE EXCHANGE INTEGRALS FOR CYCLOPHANE-TYPE CARBENE DIMERS. Chemistry Letters, 1986, 15, 625-628.	1.3	201
14	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.	3.3	176
15	Ab initio molecular orbital calculations of effective exchange integrals between transition metal ions. Chemical Physics Letters, 1988, 143, 371-376.	2.6	154
16	Theoretical studies on effective spin interactions, spin alignments and macroscopic spin tunneling in polynuclear manganese and related complexes and their mesoscopic clusters. Coordination Chemistry Reviews, 2000, 198, 265-295.	18.8	133
17	Theoretical Approaches to Direct Exchange Couplings between Divalent Chromium Ions in Naked Dimers, Tetramers, and Clusters. Journal of Physical Chemistry A, 1997, 101, 705-712.	2.5	132
18	Approximately spin-projected geometry optimization method and its application to di-chromium systems. Chemical Physics Letters, 2007, 442, 445-450.	2.6	129

#	Article	IF	Citations
19	Analytical and ab initio studies of effective exchange interactions, polyradical character, unpaired electron density, and information entropy in radical clusters (R)N: Allyl radical cluster (N=2-10) and hydrogen radical cluster (N=50). International Journal of Quantum Chemistry, 2002, 90, 370-385.	2.0	122
20	A generalized MO (GMO) approach to unstable molecules with quasi-degenerate electronic states: GMO calculations of intramolecular effective exchange integrals and designing of organic magnetic polymers. Synthetic Metals, 1987, 19, 81-86.	3.9	109
21	Density functional study of intramolecular ferromagnetic interaction throughm-phenylene coupling unit (I): UBLYP, UB3LYP, and UHF calculations. Journal of Chemical Physics, 2000, 113, 4035-4051.	3.0	105
22	A molecular-orbital theoretical classification of reactions of singlet ground-state molecules. Chemical Physics Letters, 1973, 22, 461-465.	2.6	103
23	Possibilities of organic ferromagnets and ferrimagnets by the use of charge-transfer (CT) complexes with radical substituents. Ab initio MO studies. Chemical Physics Letters, 1990, 166, 408-414.	2.6	98
24	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.	2.6	96
25	Antiferromagnetic coupling of transition metal spins across pyrimidine and pyrazine bridges in dinuclear manganese(ii), cobalt(ii), nickel(ii) and copper(ii) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate complexes. Dalton Transactions RSC, 2002, , 3177-3186.	2.3	91
26	Chemical Equilibrium Models for the S₃ State of the Oxygen-Evolving Complex of Photosystem II. Inorganic Chemistry, 2016, 55, 502-511.	4.0	90
27	Electronic structures of antiaromatic molecules. Chemical Physics Letters, 1975, 35, 230-235.	2.6	88
28	EHF theory of chemical reactions Part 4. UNO CASSCF, UNO CASPT2 and R(U)HF coupled-cluster (CC) wavefunctions. Journal of Molecular Structure, 1994, 310, 205-218.	3.6	87
29	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.	2.6	79
30	Many-electron hyperpolarizability density analysis: Application to the dissociation processof one-dimensionalH2s. Physical Review A, 1997, 55, 1503-1513.	2.5	76
31	Through-Bond and Long-Range Ferromagnetic Spin Alignment in a .pi.-Conjugated Polyradical with a Poly(phenylenevinylene) Skeleton. Journal of the American Chemical Society, 1995, 117, 548-549.	13.7	75
32	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.	7.1	69
33	Symmetry and broken symmetries in molecular orbital descriptions of unstable molecules II. Alignment, flustration and tunneling of spins in mesoscopic molecular magnets. Theoretical Chemistry Accounts, 1999, 102, 328-345.	1.4	68
34	Extended Hartreeâ€"Fock (EHF) theory of chemical reactions VI: hybrid DFT and post-Hartreeâ€"Fock approaches for concerted and non-concerted transition structures of the Dielsâ€"Alder reaction. Molecular Physics, 2002, 100, 717-727.	1.7	68
35	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A1) by Broken-Symmetry Method. Journal of Physical Chemistry A, 2009, 113, 15041-15046.	2.5	68
36	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.	2.6	66

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37	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.	2.0	66
38	Antiferromagnetic spin couplings between iron ions in ironâ€"sulfur clusters. A localized picture by the spin vector model. Chemical Physics Letters, 1989, 164, 210-216.	2.6	63
39	Extended Hartree-Fock (EHF) theory in chemical reactions. Theoretica Chimica Acta, 1978, 48, 185-206.	0.8	61
40	Singlet unrestricted Hartree-Fock Slater (UHFS) model for unstable metalî—¸metal bonds. Chemical Physics Letters, 1979, 66, 395-399.	2.6	60
41	A formulation and numerical approach to molecular systems by the Green function method without the Bornâ€"Oppenheimer approximation. Journal of Chemical Physics, 1999, 111, 6171-6179.	3.0	60
42	Theoretical study of the magnetic interaction for Mâ€"Oâ€"M type metal oxides. Comparison of broken-symmetry approaches. Polyhedron, 2001, 20, 1177-1184.	2.2	60
43	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.	2.0	60
44	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.	2.0	60
45	General spin structures of organic radicals. Chemical Physics Letters, 1975, 30, 288-292.	2.6	58
46	Electronic and spin structures of manganese clusters in the photosynthesis II system. Polyhedron, 2005, 24, 2767-2777.	2.2	58
47	Ab initio UHF and UHF NO CI approaches for quasi-degenerate systems: methylene peroxide (CH2OO). Chemical Physics Letters, 1980, 71, 563-568.	2.6	57
48	Density-functional study of intramolecular ferromagnetic interaction throughm-phenylene coupling unit (II): Examination of functional dependence. Journal of Chemical Physics, 2000, 113, 10486-10504.	3.0	57
49	CAS-DFT based on odd-electron density and radical density. Chemical Physics Letters, 2002, 366, 321-328.	2.6	56
50	Magnetic Properties of Oxygen Physisorbed in Cu-Trans-1,4-Cyclohexanedicarboxylic Acid. Molecular Crystals and Liquid Crystals, 1997, 306, 1-7.	0.3	55
51	Configuration interaction (CI), coupled-cluster (CC) and many-body perturbation (MBPT) approaches in the unrestricted Hartreeâ€"Fockâ€"Slater (UHFS) model. Chemical Physics Letters, 1979, 68, 477-482.	2.6	54
52	Density functional theory without the Born-Oppenheimer approximation and its application. International Journal of Quantum Chemistry, 1998, 70, 659-669.	2.0	54
53	Potential energy curves for transition metal dimers and complexes calculated by the approximately projected unrestricted Hartree-Fock and MÃ¸ller-Plesset perturbation (APUMP) methods. Chemical Physics Letters, 1989, 158, 95-101.	2.6	53
54	CASSCF and CASPT2 calculations of hole-doped polycarbenes. Possibilities of organic ferromagnetic conductors and metals. Chemical Physics Letters, 1995, 233, 257-265.	2.6	52

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55	Mechanisms of the reactions of singlet molecular oxygen with olefins. Chemical Physics Letters, 1973, 22, 466-470.	2.6	51
56	Interrelationships between the effective for the H3 radical. Chemical Physics Letters, 1977, 46, 360-365.	2.6	51
57	N-band Hubbard models for copper oxides and isoelectronic systems. New models for organic and organometallic magnetic conductors and superconductors. International Journal of Quantum Chemistry, 1990, 37, 167-196.	2.0	51
58	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.	2.6	51
59	Geometry optimization of the ring-opened oxirane diradical: mechanism of the addition reaction of the triplet oxygen atom to olefins. Chemical Physics Letters, 1980, 70, 27-30.	2.6	50
60	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.	7.1	50
61	Generalized Hartree-Fock natural-orbital configuration-interaction (GHF NO CI) approach to unstable molecules: trimethylene. Chemical Physics Letters, 1977, 49, 555-559.	2.6	49
62	Theory of chemical bonds in metalloenzymes I: Analytical and hybrid-DFT studies on oxo and hydroxo diiron cores. International Journal of Quantum Chemistry, 2004, 100, 887-906.	2.0	49
63	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.	2.0	49
64	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.	4.1	49
65	New models for organic magnetic conductors or organic kondo and dense kondo systems. Synthetic Metals, 1991, 43, 3631-3634.	3.9	48
66	Density functional study of intramolecular ferromagnetic interaction through m-phenylene coupling unit. III. Possibility of high-spin polymer. Journal of Chemical Physics, 1999, 111, 1309-1324.	3.0	48
67	Theory of chemical bonds in metalloenzymes VI: Manganeseâ€“oxo bonds in the photosynthesis II system. Polyhedron, 2007, 26, 2216-2224.	2.2	48
68	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, 321-343.	2.0	48
69	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.	2.8	48
70	Possibilities of charge- and/or spin-mediated superconductors and photo-induced superconductors in the intermediate region of metal-insulator transitions. International Journal of Quantum Chemistry, 1997, 65, 947-964.	2.0	47
71	Mechanistic characterization of the thermal ring-opening of three-membered cyclic compounds. Chemical Physics Letters, 1973, 22, 471-475.	2.6	44
72	Symmetry and broken symmetry in molecular orbital (MO) descriptions of unstable molecules. Generalized MO theoretical studies on 1,3-dipolar species. Computational and Theoretical Chemistry, 1983, 103, 101-120.	1.5	44

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73	Generalized spin density functional theory for noncollinear molecular magnetism. International Journal of Quantum Chemistry, 2000, 80, 664-671.	2.0	44
74	The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and ?-oxo-bridged manganese porphyrin dimer. International Journal of Quantum Chemistry, 2004, 100, 943-956.	2.0	42
75	Generalized molecular orbital (GMO) theories of organic reaction mechanisms. Orbital symmetry, orbital stability and orbital pairing rules. Chemical Physics, 1978, 29, 117-139.	1.9	41
76	Preparation and Magnetic Properties of Mn(hfac)2-Complexes of 2-(5-Pyrimidinyl)- and 2-(3-Pyridyl)-Substituted Nitronyl Nitroxides. Inorganic Chemistry, 2003, 42, 3221-3228.	4.0	41
77	Extended Hubbard Models for Transition Metal Oxides and Halides: Importance of Spin and Charge Fluctuations in Charge Transfer Metals. Japanese Journal of Applied Physics, 1988, 27, L1835-L1838.	1.5	40
78	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.	1.4	40
79	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.	5.3	40
80	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. Chemical Physics Letters, 1994, 226, 372-380.	2.6	39
81	Theoretical studies on the magnetic interaction and reversible dioxygen binding of the active site in hemocyanin. Chemical Physics Letters, 2001, 335, 395-403.	2.6	38
82	Water Oxidation Chemistry of a Synthetic Dinuclear Ruthenium Complex Containing Redox-Active Quinone Ligands. Inorganic Chemistry, 2014, 53, 3973-3984.	4.0	38
83	Selection rule in free radical reactions. Chemical Physics Letters, 1974, 28, 93-97.	2.6	37
84	EHF theory of chemical reactions V. Nature of manganese-oxygen bonds by hybrid density functional theory (DFT) and coupled-cluster (CC) methods. International Journal of Quantum Chemistry, 2001, 85, 34-43.	2.0	37
85	and semiempirical MO calculations of intermolecular effective exchange integrals between organic radicals. Designing of organic ferromagnet, ferrimagnet and ferromagnetic conductors. Synthetic Metals, 1987, 19, 87-92.	3.9	36
86	Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. International Journal of Quantum Chemistry, 2001, 84, 592-600.	2.0	36
87	Instability in chemical bonds. II. Theoretical studies of exchange-coupled open-shell systems. International Journal of Quantum Chemistry, 1993, 48, 501-515.	2.0	35
88	Heisenberg models of radical reactions: Local spin (magnetic) symmetry conservations of biradical species. Chemical Physics, 1977, 20, 171-181.	1.9	34
89	Multireference density functional theory with orbital-dependent correlation corrections. International Journal of Quantum Chemistry, 2006, 106, 3312-3324.	2.0	33
90	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.	2.0	33

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91	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.	1.7	33
92	Correlation effects in singlet biradical species. Chemical Physics, 1977, 19, 35-42.	1.9	32
93	Approximately projected UHF MÃ¸ller-Plesset calculations of the potential energy profiles for the reaction of the triplet oxygen atom with ethylene. Chemical Physics Letters, 1990, 167, 291-297.	2.6	32
94	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.	2.0	32
95	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.	1.2	32
96	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.	0.8	32
97	Theoretical studies on anomalous phases of photodoped systems in two-band model. Journal of Chemical Physics, 2000, 113, 11237-11244.	3.0	31
98	Density functional study of tetrahedral manganese clusters. Polyhedron, 2003, 22, 2013-2017.	2.2	31
99	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.	3.2	31
100	Spin contamination errors on spin-polarized density functional theory/plane-wave calculations for crystals of one-dimensional materials. Applied Physics Express, 2019, 12, 115506.	2.4	31
101	Ab initio MO Studies on the Correlation and Spin Correlation Effects for Copper-Oxygen and Copper-Halogen Bonds in High-TcCopper Oxide Superconductors. Japanese Journal of Applied Physics, 1987, 26, L2037-L2040.	1.5	30
102	CASSCF and CASPT2 calculations of hole-doped amines with triplet carbene groups. Possibilities of high-Tc organic ferrimagnets. Chemical Physics Letters, 1995, 233, 88-94.	2.6	30
103	CASSCF, MP2, and CASMP2 studies on addition reaction of singlet molecular oxygen to ethylene molecule. International Journal of Quantum Chemistry, 1997, 65, 787-801.	2.0	30
104	Singletâ€“triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. Theoretical Chemistry Accounts, 2011, 130, 739-748.	1.4	30
105	A general spin-orbital (GSO) description of antiferromagnetic spin couplings between four irons in iron-sulfur clusters. Chemical Physics Letters, 1990, 168, 56-62.	2.6	29
106	High-spin ion radicals of polyenes and polyamines. A MO theoretical study. Chemical Physics Letters, 1993, 207, 9-14.	2.6	29
107	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.	2.6	29
108	Possible Organic Analogues to Copper Oxides: Applications of a J-Model. Japanese Journal of Applied Physics, 1988, 27, L766-L769.	1.5	28

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109	Density functional and post-Hartree-Fock studies on effective exchange interaction ofd-?-d conjugated systems involvingm-phenylene-type bridge. International Journal of Quantum Chemistry, 2000, 80, 681-691.	2.0	28
110	Approximate on-top pair density into one-body functions for CAS-DFT. International Journal of Quantum Chemistry, 2004, 96, 463-473.	2.0	28
111	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.	2.0	28
112	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.	1.7	28
113	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.	2.6	28
114	Theoretical Studies on Magnetic Interactions in Prussian Blue Analogs and Active Controls of Spin States by External Fields. Molecular Crystals and Liquid Crystals, 1997, 305, 109-128.	0.3	27
115	Theoretical calculations of effective exchange integrals by spin projected and unprojected broken-symmetry methods. I. Cluster models of K2NiF4-type solids. Journal of Chemical Physics, 2003, 118, 9747-9761.	3.0	27
116	On the mechanisms of aromatic substitution reactions. Chemical Physics Letters, 1976, 44, 65-69.	2.6	26
117	Theoretical Studies of Magnetic Orderings in the Î²- and Î³-Phases of P-NPNN and Related Nitroxides. Molecular Crystals and Liquid Crystals, 1993, 232, 35-44.	0.3	26
118	Theoretical studies on anomalous phases in molecular systems with external field: Possibility of photo-induced superconductivity. International Journal of Quantum Chemistry, 1999, 75, 549-561.	2.0	26
119	Instability of a system and its estimation in terms of the hybrid density functional theory method: a magnetic effective density functional (MEDF) approach. Molecular Physics, 2002, 100, 1829-1838.	1.7	26
120	Ab Initio Extended Density Functional Theory for Strongly Correlated Electron Systems: Fundamental Aspects of the Broken-Symmetry Approach and Possible Applications for Molecular Material Design. Bulletin of the Chemical Society of Japan, 2004, 77, 1269-1286.	3.2	26
121	Quantum spin correction scheme for ab initio spin-unrestricted solutions: Multiple bonds case. International Journal of Quantum Chemistry, 2005, 105, 605-614.	2.0	26
122	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.	2.6	26
123	Ab Initio Size-Consistent Calculations of Effective Exchange Interactions in Mesoscopic Magnetic Clusters Composed of Triplet Methylenes and Quartet Nitrogen Atoms. Bulletin of the Chemical Society of Japan, 1998, 71, 2097-2108.	3.2	25
124	Synthesis and Gas-Occlusion Properties of Ruthenium(II,III) Dicarboxylates (Fumarate,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (<i>Liquid Crystals, 2000, 342, 199-204.	0.3	25
125	Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron-sulfur clusters. International Journal of Quantum Chemistry, 2005, 105, 628-644.	2.0	25
126	Recent Development of Multireference Density Functional Theory. Chemistry Letters, 2006, 35, 242-247.	1.3	25

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127	Geometric and electronic structures of the synthetic Mn₄CaO₄ model compound mimicking the photosynthetic oxygen-evolving complex. Physical Chemistry Chemical Physics, 2016, 18, 11330-11340.	2.8	25
128	Ab initio unrestricted Hartree-Fock (UHF) andUHF-natural orbitalCI studies of ozone. International Journal of Quantum Chemistry, 1980, 18, 101-106.	2.0	24
129	Spin-mediated superconductivity in cuprates, organic conductors and Ï€â€“d conjugated systems. Coordination Chemistry Reviews, 2002, 226, 235-249.	18.8	24
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.	2.0	24
131	Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Feâ€4S clusters. International Journal of Quantum Chemistry, 2008, 108, 2881-2887.	2.0	24
132	Theoretical studies of free radical reactions IV. Selection rules. Chemical Physics, 1977, 25, 215-235.	1.9	23
133	Localized natural orbitals of unstable molecules: ozone. Chemical Physics Letters, 1977, 50, 266-270.	2.6	23
134	Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order Mï¿½ller-Plesset perturbation theory level based on the quasi-energy derivative method. International Journal of Quantum Chemistry, 1997, 65, 665-677.	2.0	23
135	Local magnetic structure due to inhomogeneity of interaction inS=12antiferromagnetic chains. Physical Review B, 2000, 61, 4033-4040.	3.2	23
136	Unique Structural and Electronic Features of Perferrylâ€“Oxo Oxidant in Cytochrome P450. Journal of Physical Chemistry B, 2011, 115, 10730-10738.	2.6	23
137	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.	0.8	23
138	Synthesis and Characterization of Novel Inclusion Complexes between Microporous Molybdenum(II) Dicarboxylates and Organic Polymers. Macromolecules, 2000, 33, 6222-6227.	4.8	22
139	6-Oxophenalenoxyl derivatives covalently linked to TTF moieties: synthesis, ESR/ENDOR measurements, and DFT calculations. Tetrahedron Letters, 2001, 42, 7991-7995.	1.4	22
140	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.	2.6	22
141	Heisenberg models of radical reactions. Theoretica Chimica Acta, 1977, 45, 1-20.	0.8	21
142	DODS natural orbital (NO) CI investigations of 1,3â€diradicals: CH2NHO, CH2OO, and CH2CH2O. Journal of Chemical Physics, 1978, 68, 4323-4325.	3.0	21
143	Intermolecular Ferromagnetic Interaction of 4-(1-Pyrenylmethyleneamino)-2,2,6,6-Tetra Methylpiperidin-1-Oxyl. Molecular Crystals and Liquid Crystals, 1993, 232, 99-102.	0.3	21
144	Density functional investigation on the ferromagnetic coupling of spins in phenylenevinylene-bridged nitroxide radicals: Monomer and polymer cases. Journal of Chemical Physics, 1999, 111, 2283-2294.	3.0	21

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145	Density functional study of manganese dimer. International Journal of Quantum Chemistry, 2007, 107, 3178-3190.	2.0	21
146	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.	2.0	21
147	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.	2.6	21
148	Electron-transfer biradical intermediates in ground-state reactions. Chemical Physics Letters, 1976, 40, 347-352.	2.6	20
149	Density functional theory without the Born-Oppenheimer approximation. II. Green function techniques. International Journal of Quantum Chemistry, 1999, 75, 875-883.	2.0	20
150	Noncollinear spin density functional theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 670-676.	2.0	20
151	Generalized spin density functional theory for noncollinear molecular magnetism II?Influence of gradient correction and self-interaction correction. International Journal of Quantum Chemistry, 2001, 85, 421-431.	2.0	20
152	Hybrid DFT study of electronic structure on quasi-one-dimensional halogen-bridged binuclear metal complexes (MMX). Polyhedron, 2003, 22, 2027-2038.	2.2	20
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