

Kizashi Yamaguchi

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4507837/publications.pdf>

Version: 2024-02-01

433
papers

12,834
citations

34100

52
h-index

38392

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 M \ddot{A} ller-Plesset wavefunctions for singlet diradicals and polyradicals. <i>Chemical Physics Letters</i> , 1988, 149, 537-542.	2.6	720
2	Ab initio computations of effective exchange integrals for H $\hat{\epsilon}$ H, H $\hat{\epsilon}$ He $\hat{\epsilon}$ H and Mn ₂ O ₂ complex: comparison of broken-symmetry approaches. <i>Chemical Physics Letters</i> , 2000, 319, 223-230.	2.6	675
3	The electronic structures of biradicals in the unrestricted Hartree-Fock approximation. <i>Chemical Physics Letters</i> , 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. <i>Journal of the American Chemical Society</i> , 1998, 120, 12686-12687.	13.7	352
5	Effective exchange integrals for open-shell species by density functional methods. <i>Chemical Physics Letters</i> , 1994, 231, 25-33.	2.6	304
6	Distribution of odd electrons in ground-state molecules. <i>Theoretica Chimica Acta</i> , 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. <i>Chemical Physics Letters</i> , 2006, 432, 343-347.	2.6	268
9	Size $\hat{\epsilon}$ consistent approach and density analysis of hyperpolarizability: Second hyperpolarizabilities of polymeric systems with and without defects. <i>Journal of Chemical Physics</i> , 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. <i>Science</i> , 2019, 366, 334-338.	12.6	248
11	Extended Hartree-Fock (EHF) theory of chemical reactions. <i>Theoretica Chimica Acta</i> , 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. <i>Japanese Journal of Applied Physics</i> , 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. <i>Chemistry Letters</i> , 1986, 15, 625-628.	1.3	201
14	Theoretical illumination of water-inserted structures of the CaMn ₄ O ₅ cluster in the S ₂ and S ₃ states of oxygen-evolving complex of photosystem II: full geometry optimizations by B3LYP hybrid density functional. <i>Dalton Transactions</i> , 2012, 41, 13727.	3.3	176
15	Ab initio molecular orbital calculations of effective exchange integrals between transition metal ions. <i>Chemical Physics Letters</i> , 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. <i>Coordination Chemistry Reviews</i> , 2000, 198, 265-295.	18.8	133
17	Theoretical Approaches to Direct Exchange Couplings between Divalent Chromium Ions in Naked Dimers, Tetramers, and Clusters. <i>Journal of Physical Chemistry A</i> , 1997, 101, 705-712.	2.5	132
18	Approximately spin-projected geometry optimization method and its application to di-chromium systems. <i>Chemical Physics Letters</i> , 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). <i>International Journal of Quantum Chemistry</i> , 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. <i>Synthetic Metals</i> , 1987, 19, 81-86.	3.9	109
21	Density functional study of intramolecular ferromagnetic interaction through-phenylene coupling unit (I): UBLYP, UB3LYP, and UHF calculations. <i>Journal of Chemical Physics</i> , 2000, 113, 4035-4051.	3.0	105
22	A molecular-orbital theoretical classification of reactions of singlet ground-state molecules. <i>Chemical Physics Letters</i> , 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. <i>Chemical Physics Letters</i> , 1990, 166, 408-414.	2.6	98
24	Possible mechanisms for the O-H bond formation in oxygen evolution reaction at the CaMn ₄ O ₅ (H ₂ O) ₄ cluster of PSII refined to 1.9 Å... X-ray resolution. <i>Chemical Physics Letters</i> , 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. <i>Dalton Transactions RSC</i> , 2002, , 3177-3186.	2.3	91
26	Chemical Equilibrium Models for the S ₃ State of the Oxygen-Evolving Complex of Photosystem II. <i>Inorganic Chemistry</i> , 2016, 55, 502-511.	4.0	90
27	Electronic structures of antiaromatic molecules. <i>Chemical Physics Letters</i> , 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. <i>Journal of Molecular Structure</i> , 1994, 310, 205-218.	3.6	87
29	QM/MM study of the S ₂ to S ₃ transition reaction in the oxygen-evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 2015, 636, 172-179.	2.6	79
30	Many-electron hyperpolarizability density analysis: Application to the dissociation process of one-dimensional H ₂ s. <i>Physical Review A</i> , 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. <i>Journal of the American Chemical Society</i> , 1995, 117, 548-549.	13.7	75
32	Structure and function of a hexameric copper-containing nitrite reductase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 4315-4320.	7.1	69
33	Symmetry and broken symmetries in molecular orbital descriptions of unstable molecules II. Alignment, frustration and tunneling of spins in mesoscopic molecular magnets. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 328-345.	1.4	68
34	Extended Hartree-Fock (EHF) theory of chemical reactions VI: hybrid DFT and post-Hartree-Fock approaches for concerted and non-concerted transition structures of the Diels-Alder reaction. <i>Molecular Physics</i> , 2002, 100, 717-727.	1.7	68
35	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A ₁) by Broken-Symmetry Method. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15041-15046.	2.5	68
36	Labile electronic and spin states of the CaMn ₄ O ₅ cluster in the PSII system refined to the 1.9 Å... X-ray resolution. UB3LYP computational results. <i>Chemical Physics Letters</i> , 2011, 506, 98-103.	2.6	66

#	ARTICLE	IF	CITATIONS
37	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn_4O_5 cluster of PSII refined to 1.9 Å... X-ray resolution. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 253-276.	2.0	66
38	Antiferromagnetic spin couplings between iron ions in iron-sulfur clusters. A localized picture by the spin vector model. <i>Chemical Physics Letters</i> , 1989, 164, 210-216.	2.6	63
39	Extended Hartree-Fock (EHF) theory in chemical reactions. <i>Theoretica Chimica Acta</i> , 1978, 48, 185-206.	0.8	61
40	Singlet unrestricted Hartree-Fock Slater (UHFS) model for unstable metal-metal bonds. <i>Chemical Physics Letters</i> , 1979, 66, 395-399.	2.6	60
41	A formulation and numerical approach to molecular systems by the Green function method without the Born-Oppenheimer approximation. <i>Journal of Chemical Physics</i> , 1999, 111, 6171-6179.	3.0	60
42	Theoretical study of the magnetic interaction for $\text{M}^{\text{O}}\text{M}$ type metal oxides. Comparison of broken-symmetry approaches. <i>Polyhedron</i> , 2001, 20, 1177-1184.	2.2	60
43	Full geometry optimizations of the mixed-valence $\text{CaMn}_4\text{O}_4\text{X}(\text{H}_2\text{O})_4$ ($\text{X}=\text{OH}$ or O) cluster in OEC of PS II: Degree of symmetry breaking of the labile Mn-X-Mn bond revealed by several hybrid DFT calculations. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 525-541.	2.0	60
44	The nature of chemical bonds of the CaMn_4O_5 cluster in oxygen evolving complex of photosystem II: Jahn-Teller distortion and its suppression by Ca doping in cubane structures. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 453-473.	2.0	60
45	General spin structures of organic radicals. <i>Chemical Physics Letters</i> , 1975, 30, 288-292.	2.6	58
46	Electronic and spin structures of manganese clusters in the photosynthesis II system. <i>Polyhedron</i> , 2005, 24, 2767-2777.	2.2	58
47	Ab initio UHF and UHF NO CI approaches for quasi-degenerate systems: methylene peroxide (CH_2OO). <i>Chemical Physics Letters</i> , 1980, 71, 563-568.	2.6	57
48	Density-functional study of intramolecular ferromagnetic interaction through m -phenylene coupling unit (II): Examination of functional dependence. <i>Journal of Chemical Physics</i> , 2000, 113, 10486-10504.	3.0	57
49	CAS-DFT based on odd-electron density and radical density. <i>Chemical Physics Letters</i> , 2002, 366, 321-328.	2.6	56
50	Magnetic Properties of Oxygen Physisorbed in Cu-Trans-1,4-Cyclohexanedicarboxylic Acid. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 1-7.	0.3	55
51	Configuration interaction (CI), coupled-cluster (CC) and many-body perturbation (MBPT) approaches in the unrestricted Hartree-Fock Slater (UHFS) model. <i>Chemical Physics Letters</i> , 1979, 68, 477-482.	2.6	54
52	Density functional theory without the Born-Oppenheimer approximation and its application. <i>International Journal of Quantum Chemistry</i> , 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 Møller-Plesset perturbation (APUMP) methods. <i>Chemical Physics Letters</i> , 1989, 158, 95-101.	2.6	53
54	CASSCF and CASPT2 calculations of hole-doped polycarbenes. Possibilities of organic ferromagnetic conductors and metals. <i>Chemical Physics Letters</i> , 1995, 233, 257-265.	2.6	52

#	ARTICLE	IF	CITATIONS
55	Mechanisms of the reactions of singlet molecular oxygen with olefins. <i>Chemical Physics Letters</i> , 1973, 22, 466-470.	2.6	51
56	Interrelationships between the effective for the H3 radical. <i>Chemical Physics Letters</i> , 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. <i>International Journal of Quantum Chemistry</i> , 1990, 37, 167-196.	2.0	51
58	Strong Coupling between the Hydrogen Bonding Environment and Redox Chemistry during the $S_{2\rightarrow 3}$ Transition in the Oxygen-Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry B</i> , 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. <i>Chemical Physics Letters</i> , 1980, 70, 27-30.	2.6	50
60	Similarities of artificial photosystems by ruthenium oxo complexes and native water splitting systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15600-15605.	7.1	50
61	Generalized Hartree-Fock natural-orbital configuration-interaction (GHF NO CI) approach to unstable molecules: trimethylene. <i>Chemical Physics Letters</i> , 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. <i>International Journal of Quantum Chemistry</i> , 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. <i>International Journal of Quantum Chemistry</i> , 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 Mn-Mn distances with hydrogen bonds. <i>Catalysis Science and Technology</i> , 2013, 3, 1831.	4.1	49
65	New models for organic magnetic conductors or organic kondo and dense kondo systems. <i>Synthetic Metals</i> , 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. <i>Journal of Chemical Physics</i> , 1999, 111, 1309-1324.	3.0	48
67	Theory of chemical bonds in metalloenzymes VI: Manganese-oxo bonds in the photosynthesis II system. <i>Polyhedron</i> , 2007, 26, 2216-2224.	2.2	48
68	Structure and reactivity of the mixed-valence $CaMn_4O_5(H_2O)_4$ and $CaMn_4O_4(OH)(H_2O)_4$ clusters at oxygen evolution complex of photosystem II. Hybrid DFT (UB3LYP and UBHandHLYP) calculations. <i>International Journal of Quantum Chemistry</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 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. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 947-964.	2.0	47
71	Mechanistic characterization of the thermal ring-opening of three-membered cyclic compounds. <i>Chemical Physics Letters</i> , 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. <i>Computational and Theoretical Chemistry</i> , 1983, 103, 101-120.	1.5	44

#	ARTICLE	IF	CITATIONS
73	Generalized spin density functional theory for noncollinear molecular magnetism. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 664-671.	2.0	44
74	The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and μ -oxo-bridged manganese porphyrin dimer. <i>International Journal of Quantum Chemistry</i> , 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. <i>Chemical Physics</i> , 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. <i>Inorganic Chemistry</i> , 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. <i>Japanese Journal of Applied Physics</i> , 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 antiaromatic molecules. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 749-763.	1.4	40
79	Spin, Valence, and Structural Isomerism in the $S_{3/2}$ State of the Oxygen-Evolving Complex of Photosystem II as a Manifestation of Multimetallic Cooperativity. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2375-2391.	5.3	40
80	Electronic structures of poly-cations and -anions of C ₆₀ . Possible mechanisms of organic ferromagnetism. <i>Chemical Physics Letters</i> , 1994, 226, 372-380.	2.6	39
81	Theoretical studies on the magnetic interaction and reversible dioxygen binding of the active site in hemocyanin. <i>Chemical Physics Letters</i> , 2001, 335, 395-403.	2.6	38
82	Water Oxidation Chemistry of a Synthetic Dinuclear Ruthenium Complex Containing Redox-Active Quinone Ligands. <i>Inorganic Chemistry</i> , 2014, 53, 3973-3984.	4.0	38
83	Selection rule in free radical reactions. <i>Chemical Physics Letters</i> , 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. <i>International Journal of Quantum Chemistry</i> , 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. <i>Synthetic Metals</i> , 1987, 19, 87-92.	3.9	36
86	Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 592-600.	2.0	36
87	Instability in chemical bonds. II. Theoretical studies of exchange-coupled open-shell systems. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 501-515.	2.0	35
88	Heisenberg models of radical reactions: Local spin (magnetic) symmetry conservations of biradical species. <i>Chemical Physics</i> , 1977, 20, 171-181.	1.9	34
89	Multireference density functional theory with orbital-dependent correlation corrections. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3312-3324.	2.0	33
90	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Fe-2S] cluster. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 116-133.	2.0	33

#	ARTICLE	IF	CITATIONS
91	Theory of chemical bonds in metalloenzymes XXI. Possible mechanisms of water oxidation in oxygen evolving complex of photosystem II. <i>Molecular Physics</i> , 2018, 116, 717-745.	1.7	33
92	Correlation effects in singlet biradical species. <i>Chemical Physics</i> , 1977, 19, 35-42.	1.9	32
93	Approximately projected UHF Møller-Plesset calculations of the potential energy profiles for the reaction of the triplet oxygen atom with ethylene. <i>Chemical Physics Letters</i> , 1990, 167, 291-297.	2.6	32
94	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Fe μ -S ₂] clusters. <i>International Journal of Quantum Chemistry</i> , 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. <i>Supramolecular Chemistry</i> , 2011, 23, 287-296.	1.2	32
96	Electronic and Spin Structures of the CaMn ₄ O ₅ (H ₂ O) ₄ Cluster in OEC of PSII Refined to 1.9Å... X-ray Resolution. <i>Advances in Quantum Chemistry</i> , 2012, 64, 121-187.	0.8	32
97	Theoretical studies on anomalous phases of photodoped systems in two-band model. <i>Journal of Chemical Physics</i> , 2000, 113, 11237-11244.	3.0	31
98	Density functional study of tetrahedral manganese clusters. <i>Polyhedron</i> , 2003, 22, 2013-2017.	2.2	31
99	Large-scale QM/MM calculations of the CaMn ₄ O ₅ cluster in the S ₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. <i>Faraday Discussions</i> , 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. <i>Applied Physics Express</i> , 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-Tc Copper Oxide Superconductors. <i>Japanese Journal of Applied Physics</i> , 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. <i>Chemical Physics Letters</i> , 1995, 233, 88-94.	2.6	30
103	CASSCF, MP2, and CASMP2 studies on addition reaction of singlet molecular oxygen to ethylene molecule. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 787-801.	2.0	30
104	Singlet-triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. <i>Theoretical Chemistry Accounts</i> , 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. <i>Chemical Physics Letters</i> , 1990, 168, 56-62.	2.6	29
106	High-spin ion radicals of polyenes and polyamines. A MO theoretical study. <i>Chemical Physics Letters</i> , 1993, 207, 9-14.	2.6	29
107	Theoretical studies of the damage-free S ₁ structure of the CaMn ₄ O ₅ cluster in oxygen-evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 2015, 623, 1-7.	2.6	29
108	Possible Organic Analogues to Copper Oxides: Applications of a J-Model. <i>Japanese Journal of Applied Physics</i> , 1988, 27, L766-L769.	1.5	28

#	ARTICLE	IF	CITATIONS
109	Density functional and post-Hartree-Fock studies on effective exchange interaction of d - d conjugated systems involving m -phenylene-type bridge. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 681-691.	2.0	28
110	Approximate on-top pair density into one-body functions for CAS-DFT. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 463-473.	2.0	28
111	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic $[8Fe\mu_4S]$ core. <i>International Journal of Quantum Chemistry</i> , 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. <i>Molecular Physics</i> , 2015, 113, 359-384.	1.7	28
113	Nonadiabatic one-electron transfer mechanism for the O-O bond formation in the oxygen-evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 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. <i>Molecular Crystals and Liquid Crystals</i> , 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 K_2NiF_4 -type solids. <i>Journal of Chemical Physics</i> , 2003, 118, 9747-9761.	3.0	27
116	On the mechanisms of aromatic substitution reactions. <i>Chemical Physics Letters</i> , 1976, 44, 65-69.	2.6	26
117	Theoretical Studies of Magnetic Orderings in the \hat{I}^2 - and \hat{I}^3 -Phases of P-NPNN and Related Nitroxides. <i>Molecular Crystals and Liquid Crystals</i> , 1993, 232, 35-44.	0.3	26
118	Theoretical studies on anomalous phases in molecular systems with external field: Possibility of photo-induced superconductivity. <i>International Journal of Quantum Chemistry</i> , 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. <i>Molecular Physics</i> , 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. <i>Bulletin of the Chemical Society of Japan</i> , 2004, 77, 1269-1286.	3.2	26
121	Quantum spin correction scheme for ab initio spin-unrestricted solutions: Multiple bonds case. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 605-614.	2.0	26
122	On the guiding principles for lucid understanding of the damage-free S1 structure of the $CaMn_4O_5$ cluster in the oxygen evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 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. <i>Bulletin of the Chemical Society of Japan</i> , 1998, 71, 2097-2108.	3.2	25
124	Synthesis and Gas-Occlusion Properties of Ruthenium(II,III) Dicarboxylates (Fumarate,) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (<i></i> <i>Liquid Crystals</i> , 2000, 342, 199-204.	0.3	25
125	Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron-sulfur clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 628-644.	2.0	25
126	Recent Development of Multireference Density Functional Theory. <i>Chemistry Letters</i> , 2006, 35, 242-247.	1.3	25

#	ARTICLE	IF	CITATIONS
127	Geometric and electronic structures of the synthetic Mn ₄ CaO ₄ model compound mimicking the photosynthetic oxygen-evolving complex. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11330-11340.	2.8	25
128	Ab initio unrestricted Hartree-Fock (UHF) and UHF-natural orbital CI studies of ozone. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 101-106.	2.0	24
129	Spin-mediated superconductivity in cuprates, organic conductors and d conjugated systems. <i>Coordination Chemistry Reviews</i> , 2002, 226, 235-249.	18.8	24
130	Geometry optimization method based on approximate spin projection and its application to F ₂ , CH ₂ , CH ₂ OO, and active site of urease. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3094-3102.	2.0	24
131	Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Fe ₄ S clusters. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2881-2887.	2.0	24
132	Theoretical studies of free radical reactions IV. Selection rules. <i>Chemical Physics</i> , 1977, 25, 215-235.	1.9	23
133	Localized natural orbitals of unstable molecules: ozone. <i>Chemical Physics Letters</i> , 1977, 50, 266-270.	2.6	23
134	Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order Møller-Plesset perturbation theory level based on the quasi-energy derivative method. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 665-677.	2.0	23
135	Local magnetic structure due to inhomogeneity of interaction in S=1/2 antiferromagnetic chains. <i>Physical Review B</i> , 2000, 61, 4033-4040.	3.2	23
136	Unique Structural and Electronic Features of Perferryl ^{IV} Oxo Oxidant in Cytochrome P450. <i>Journal of Physical Chemistry B</i> , 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 Oxidation [†] Theoretical System Models of the Oxygen-Evolving Complex of Photosystem II. <i>Advances in Quantum Chemistry</i> , 2015, 70, 325-413.	0.8	23
138	Synthesis and Characterization of Novel Inclusion Complexes between Microporous Molybdenum(II) Dicarboxylates and Organic Polymers. <i>Macromolecules</i> , 2000, 33, 6222-6227.	4.8	22
139	6-Oxophenalenoxyl derivatives covalently linked to TTF moieties: synthesis, ESR/ENDOR measurements, and DFT calculations. <i>Tetrahedron Letters</i> , 2001, 42, 7991-7995.	1.4	22
140	Role of Perferryl ^{IV} Oxo Oxidant in Alkane Hydroxylation Catalyzed by Cytochrome P450: A Hybrid Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4713-4730.	2.6	22
141	Heisenberg models of radical reactions. <i>Theoretica Chimica Acta</i> , 1977, 45, 1-20.	0.8	21
142	DODS natural orbital (NO) CI investigations of 1,3 ^π diradicals: CH ₂ NHO, CH ₂ OO, and CH ₂ CH ₂ O. <i>Journal of Chemical Physics</i> , 1978, 68, 4323-4325.	3.0	21
143	Intermolecular Ferromagnetic Interaction of 4-(1-Pyrenylmethyleneamino)-2,2,6,6-Tetra Methylpiperidin-1-Oxyl. <i>Molecular Crystals and Liquid Crystals</i> , 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. <i>Journal of Chemical Physics</i> , 1999, 111, 2283-2294.	3.0	21

#	ARTICLE	IF	CITATIONS
145	Density functional study of manganese dimer. <i>International Journal of Quantum Chemistry</i> , 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 O-H-O bond formation of water splitting reaction. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 121-135.	2.0	21
147	Concerted Mechanism of Water Insertion and O ₂ Release during the S ₄ to S ₀ Transition of the Oxygen-Evolving Complex in Photosystem II. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6491-6502.	2.6	21
148	Electron-transfer biradical intermediates in ground-state reactions. <i>Chemical Physics Letters</i> , 1976, 40, 347-352.	2.6	20
149	Density functional theory without the Born-Oppenheimer approximation. II. Green function techniques. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 875-883.	2.0	20
150	Noncollinear spin density functional theory for spin-frustrated and spin-degenerate systems. <i>International Journal of Quantum Chemistry</i> , 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. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 421-431.	2.0	20
152	Hybrid DFT study of electronic structure on quasi-one-dimensional halogen-bridged binuclear metal complexes (MMX). <i>Polyhedron</i> , 2003, 22, 2027-2038.	2.2	20
153	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of π -conjugated oligomers by intermolecular interaction. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 702-710.	2.0	20
154	Resonating broken-symmetry approach to biradicals and polyradicals. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3303-3311.	2.0	20
155	Theory of chemical bonds in metalloenzymes. VII. Hybrid density functional theory studies on the electronic structures of P450. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 631-650.	2.0	20
156	Broken-symmetry natural orbital (BSNO) MRCC study on the exchange coupling in the binuclear copper(II) compounds. <i>Chemical Physics Letters</i> , 2011, 505, 11-15.	2.6	20
157	Spin hamiltonian models for artificial and native water splitting systems revealed by hybrid DFT calculations. Oxygen activation by high-valent Mn and Ru ions. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3849-3866.	2.0	20
158	Possibility of charge-mediated superconductors in the intermediate region of metal-insulator transitions. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 1075-1084.	2.0	19
159	Theoretical investigation on the magnetic interaction of the tetrathiafulvalene-nitronyl nitroxide stacking model: possibility of organic magnetic metals and magnetic superconductors. <i>Polyhedron</i> , 2001, 20, 1169-1176.	2.2	19
160	Hybrid-density functional study of magnetism and ligand control in Ni ⁹ complexes. <i>Chemical Physics Letters</i> , 2006, 421, 483-487.	2.6	19
161	Ab initio MO Studies of the Hole Delocalization in Copper Oxides and Related Species: Necessity of the Extended Hubbard Model. <i>Japanese Journal of Applied Physics</i> , 1988, 27, L509-L512.	1.5	18
162	Ab initio molecular-orbital study on electron correlation effects in CuO ₆ clusters relating to high-T _c superconductivity. <i>Physical Review B</i> , 1990, 42, 266-272.	3.2	18

#	ARTICLE	IF	CITATIONS
163	Calculation of frequency-dependent first hyperpolarizabilities using the second-order Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 1999, 110, 11720-11733.	3.0	18
164	Size-dependency of polarizabilities of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. <i>Journal of Chemical Physics</i> , 2001, 115, 1052-1059.	3.0	18
165	Generalized spin density functional study of radical reactions. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 376-383.	2.0	18
166	CASSCF version of density functional theory. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3325-3333.	2.0	18
167	Ab initio study of magnetic interactions of manganese-oxide clusters. <i>Polyhedron</i> , 2011, 30, 3256-3261.	2.2	18
168	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional N_n ($n = 3, 5, 7$) complexes. <i>Dalton Transactions</i> , 2013, 42, 16200.	3.3	18
169	Theory of chemical bonds in metalloenzymes XIX: labile manganese oxygen bonds of the $CaMn_4O_5$ cluster in oxygen evolving complex of photosystem II. <i>Molecular Physics</i> , 2014, 112, 485-507.	1.7	18
170	Orbital symmetry, orbital stability, and orbital pairing rules for organic reactions in the ground state. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 459-484.	2.0	17
171	MP2, Tamm-Dancoff, and RPA methods based on the generalized HF solution. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 701-707.	2.0	17
172	MULTIBAND SUPERCONDUCTIVITY. <i>International Journal of Modern Physics B</i> , 2002, 16, 3419-3428.	2.0	17
173	Potential Energy Curve for Ring-Opening Reactions: Comparison Between Broken-Symmetry and Multireference Coupled Cluster Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5625-5631.	2.5	17
174	An efficient initial guess formation of broken-symmetry solutions by using localized natural orbitals. <i>Chemical Physics Letters</i> , 2014, 608, 50-54.	2.6	17
175	Concerted bond switching mechanism coupled with one-electron transfer for the oxygen-oxygen bond formation in the oxygen-evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 2019, 714, 219-226.	2.6	17
176	Theoretical Studies for Third-Order Hyperpolarizabilities of Alternant and Condensed-Ring Conjugated Systems I. <i>Molecular Crystals and Liquid Crystals</i> , 1994, 255, 139-148.	0.3	16
177	Magnetic Interaction Via \hat{I}^2 -Hydrogen Atoms in Tempo Derivatives. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 141-150.	0.3	16
178	Theoretical Study of the Antiferromagnetic Model Clusters for K_2MX_4 Type Solids. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 343, 133-138.	0.3	16
179	Spin correlation functions by generalized spin orbital density functional and multireference approaches. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 512-520.	2.0	16
180	Ab initio calculation of the Dzyaloshinskii-Moriya parameters: Spin-orbit GSO-HF, DFT, and CI approaches. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1328-1334.	2.0	16

#	ARTICLE	IF	CITATIONS
181	On the guiding principles for understanding of geometrical structures of the CaMn_4O_5 cluster in oxygen-evolving complex of photosystem II. Proposal of estimation formula of structural deformations via the Jahn-Teller effects. <i>Molecular Physics</i> , 2017, 115, 636-666.	1.7	16
182	UNO DMRG CAS CI calculations of binuclear manganese complex $\text{Mn(IV)}_2\text{O}_2(\text{NHCHCO}_2)_4$: Scope and applicability of Heisenberg model. <i>Journal of Computational Chemistry</i> , 2019, 40, 333-341.	3.3	16
183	Theoretical studies on superconducting and other phases: Triplet superconductivity, ferromagnetism, and ferromagnetic metal. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 721-732.	2.0	15
184	Local magnetic structures induced by inhomogeneities of the lattice in $S=1/2$ bond-alternating chains and their response to a time-dependent magnetic field with noise. <i>Physical Review B</i> , 2000, 62, 9463-9471.	3.2	15
185	Theoretical studies on magnetic interactions and charge-dope effects in one-dimensional Ni^{5+} and Ni^{7+} complexes. <i>Polyhedron</i> , 2005, 24, 2751-2757.	2.2	15
186	UNO and ULO MRCC (Mk), AP-UCC and AP-UBD approaches to diradical systems. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3015-3026.	2.0	15
187	Theory of chemical bonds in metalloenzymes. XIV. Correspondence between magnetic coupling mode and radical coupling mechanism in hydroxylations with methane monooxygenase and related species. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2955-2981.	2.0	15
188	Full geometry optimizations of the CaMn_4O_4 model cluster for the oxygen evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 2015, 640, 23-30.	2.6	15
189	Large-scale QM/MM calculations of the CaMn_4O_5 cluster in the oxygen-evolving complex of photosystem II: Comparisons with EXAFS structures. <i>Chemical Physics Letters</i> , 2016, 658, 354-363.	2.6	15
190	Theoretical Studies on the Magnetic and Conductive Properties of Crystals Containing Open-Shell Trioxotriangulene Radicals. <i>Bulletin of the Chemical Society of Japan</i> , 2016, 89, 315-333.	3.2	15
191	Quantum-phase and information-entropy dynamics of a two-state molecular system interacting with strongly amplitude- and phase-squeezed fields. <i>Journal of Chemical Physics</i> , 2000, 112, 2769-2780.	3.0	14
192	Generalized spin orbital calculations of spin-frustrated molecules. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 546-551.	2.0	14
193	Theoretical investigation of magnetic parameters in two-dimensional sheets of pure organic BEDT-TTF and BETS molecules by using ab initio MO and DFT methods. <i>Molecular Physics</i> , 2002, 100, 2641-2652.	1.7	14
194	Theoretical studies on ferrimagnetic behavior of TCNE and manganese porphyrin dimer. <i>Polyhedron</i> , 2005, 24, 2720-2725.	2.2	14
195	Theoretical study on the magnetic interactions of active site in hemerythrin. <i>Polyhedron</i> , 2005, 24, 2701-2707.	2.2	14
196	Extended Hartree-Fock theory of chemical reactions. VIII. Hydroxylation reactions by P450. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2991-3009.	2.0	14
197	Theoretical and computational investigations of geometrical, electronic and spin structures of the CaMn_4O_X ($X=5, 6$) cluster in the Kok cycle S_i ($i=0, 1, 2, 3$) of oxygen evolving complex of photosystem II. <i>Physiologia Plantarum</i> , 2019, 166, 44-59.	2.2	14
198	Estimation of spin contamination errors in DFT/plane-wave calculations of solid materials using approximate spin projection scheme. <i>Chemical Physics Letters</i> , 2021, 765, 138291.	2.6	14

#	ARTICLE	IF	CITATIONS
199	An ab initio molecular orbital study of a binuclear dioxygen complex as a model of the binuclear active site in cytochrome c oxidase. <i>Chemical Physics Letters</i> , 1998, 294, 459-467.	2.6	13
200	Calculation of frequency-dependent second hyperpolarizabilities for electric field induced second harmonic generation in the second-order Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 1999, 111, 842-848.	3.0	13
201	Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase and the related species. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3250-3265.	2.0	13
202	Effectiveness of Optimizing Geometry for CaMn ₄ O ₅ Cluster at 1.9 Å... Resolved OEC and Proposal for Oxidation Mechanism from S ₀ to S ₃ States. <i>Chemistry Letters</i> , 2012, 41, 18-20.	1.3	13
203	Domain-based local pair natural orbital CCSD(T) calculations of six different S ₁ structures of oxygen evolving complex of photosystem II. Proposal of multi-intermediate models for the S ₁ state. <i>Chemical Physics Letters</i> , 2019, 732, 136660.	2.6	13
204	Theoretical Elucidation of Geometrical Structures of the CaMn ₄ O ₅ Cluster in Oxygen Evolving Complex of Photosystem II Scope and Applicability of Estimation Formulae of Structural Deformations via the Mixed-Valence and Jahn-Teller Effects. <i>Advances in Quantum Chemistry</i> , 2019, , 307-451.	0.8	13
205	Zwitterionic intermediates in enamine-singlet oxygen reactions. configuration-interaction studies on the indole-singlet oxygen reactions. <i>Tetrahedron Letters</i> , 1979, 20, 3433-3436.	1.4	12
206	Zwitterionic mechanisms for photooxygenation reactions of n-activated c-c double bonds: full geometry optimizations of the diradical and zwitterionic intermediates by ab initio SCF method. <i>Chemical Physics Letters</i> , 1981, 78, 566-571.	2.6	12
207	Ab Initio Calculations of Effective Exchange Integrals. Possibilities of Superparamagnetic, Mictomagnetic and Amorphous Ferromagnetic States for Aggregates of Aromatic Free Radicals and Polymer Radicals. <i>Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics</i> , 1989, 176, 151-161.	0.3	12
208	A Two-Band Hubbard Model for Clusters of Doped Copper Oxides and Other Metal Oxides: Populations of Holes and Spin Densities by the Full VB CI Method. <i>Japanese Journal of Applied Physics</i> , 1989, 28, L479-L482.	1.5	12
209	Theoretical Approaches to Molecular Magnetism. <i>ACS Symposium Series</i> , 1996, , 30-43.	0.5	12
210	Local Magnetic Structure of Layered Compounds Cu ₂ (OD) ₃ X with Exchangeable Acid Anion X Studied by Solid State High Resolution Deuterium NMR. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 11-21.	0.3	12
211	Theoretical studies on the magnetic quantum tunneling rates in Mn clusters by the path integral method. <i>Chemical Physics Letters</i> , 1999, 302, 418-424.	2.6	12
212	A novel inclusion complex between molybdenum(II) fumarate and poly(ethylene glycol): first supramolecule formation between a microporous complex and an organic polymer. <i>Polymers for Advanced Technologies</i> , 2000, 11, 840-844.	3.2	12
213	Multireference (MR) configuration interaction (CI) approach for quasidegenerate systems. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 269-284.	2.0	12
214	Theory of chemical bonds in metalloenzymes XIII: Singlet and triplet diradical mechanisms of hydroxylations with iron-oxo species and P450 are revisited. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3723-3744.	2.0	12
215	Extended Hartree-Fock theory of chemical reactions. IX. Diradical and peroxide mechanisms for oxygenations of ethylene with molecular oxygen and iron-oxo species are revisited. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3745-3766.	2.0	12
216	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. <i>Polyhedron</i> , 2009, 28, 1945-1949.	2.2	12

#	ARTICLE	IF	CITATIONS
217	Theoretical Studies of the Ferromagnetic Inter-Molecular Interaction of P-Carboxylate Phenyl Nitronyl Nitroxide. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 279, 29-38.	0.3	11
218	Quantum-phase dynamics of dimer systems interacting with a two-mode squeezed coherent field. <i>Journal of Chemical Physics</i> , 2002, 116, 10069-10082.	3.0	11
219	Fractional occupation numbers and spin density functional calculations of degenerate systems. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 317-323.	2.0	11
220	N-band Hubbard models II: Cooperative mechanisms of electron-phonon, electron correlation, and many-band effects toward high-Tc superconductors. <i>International Journal of Quantum Chemistry</i> , 2003, 92, 47-70.	2.0	11
221	Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 615-627.	2.0	11
222	Approximately spin-projected Hessian for broken symmetry method and stretching frequencies of F_{2g} and singlet O_{2g} . <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3641-3648.	2.0	11
223	Symmetry and Broken-Symmetry in Molecular Orbital Descriptions of Unstable Molecules. 3. The Nature of Chemical Bonds of Spin Frustrated Systems. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15281-15297.	2.5	11
224	Theoretical Study on the Electronic Configurations and Nature of Chemical Bonds of Dirhodium Tetraacetato Complexes $[Rh_2(CH_3COO)_4(L)_2]$ ($L = H_2O, Free$): Broken Symmetry Approach. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 1481-1488.	3.2	11
225	MkMRCC, APUC and APUBD approaches to 1,4-didehydropolyene diradicals: the nature of through-bond exchange interactions. <i>Molecular Physics</i> , 2010, 108, 2559-2578.	1.7	11
226	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. <i>Chemical Physics Letters</i> , 2019, 734, 136731.	2.6	11
227	A Universal MO-VB Approach to Electron and Spin Correlations in Copper-Oxide Clusters: Néel Order, Spin Fluctuation and High-Tc Superconductivity. <i>Japanese Journal of Applied Physics</i> , 1988, 27, L393-L396.	1.5	10
228	Molecular Design and Synthesis of Ferro-and Ferri-Magnetic Inorganic Polymers and Complexes with Tetrathiolate Ligands. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 279, 1-8.	0.3	10
229	Theoretical Study of Effective Exchange Integrals for Ferromagnetic Phenylenevinylene Polymers with Nitroxides. Possibilities of Organic Ferro-or Ferri-Magnetic Solids. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 279, 19-28.	0.3	10
230	Hyperpolarizabilities of one-dimensional Hn systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 269-282.	2.0	10
231	CAS-SCF and density functional calculations of second hyperpolarizabilities for a nitronyl nitroxide radical. <i>International Journal of Quantum Chemistry</i> , 1999, 71, 329-336.	2.0	10
232	Possibilities of molecular magnetic metals and highTc superconductors in field effect transistor configurations. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 619-635.	2.0	10
233	Third-order nonlinear optical properties of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. <i>Journal of Chemical Physics</i> , 2001, 115, 6780-6784.	3.0	10
234	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3649-3658.	2.0	10

#	ARTICLE	IF	CITATIONS
235	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. <i>Molecular Physics</i> , 2010, 108, 2533-2541.	1.7	10
236	Approximate Spin Projection for Broken-Symmetry Method and Its Application. , 0, , .		10
237	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. <i>Chemical Physics Letters</i> , 2018, 705, 85-91.	2.6	10
238	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. <i>Chemical Physics</i> , 2019, 518, 81-90.	1.9	10
239	Clarification of the Relationship between the Magnetic and Conductive Properties of Infinite Chains in Trioxotriangulene Radical Crystals by Spin-Projected DFT/Plane-Wave Calculations. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000050.	2.8	10
240	The spin-optimized SCF general spin orbitals. Theoretical formulation. <i>Journal of Chemical Physics</i> , 1977, 67, 2527.	3.0	9
241	CNDO/S \hat{C} I Calculations of Hyperpolarizabilities. III. Regular Polyenes, Charged Polyenes, Di-substituted Polyenes, Polydiacetylene and Related Species. <i>Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics</i> , 1990, 182, 1-15.	0.3	9
242	Theoretical Calculation of Effective Exchange Integrals for One- and Two-Dimensional Poly(Phenylene-methylene) Systems. Possibilities of Organic Ferro- and Ferri-Magnetic Solids. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 279, 9-18.	0.3	9
243	Path integral method by means of generalized coherent states and its numerical approach to molecular systems. I. Ensemble average of total energy. <i>Journal of Chemical Physics</i> , 1997, 107, 6283-6289.	3.0	9
244	Theoretical Studies of Magnetic Interactions in 2,5-Dihydroxyphenyl Nitronyl Nitroxide Crystal. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 151-160.	0.3	9
245	Third-Order Nonlinear Optical Properties of a Stable Radical Species with Nitronyl Nitroxide Group. <i>Molecular Crystals and Liquid Crystals</i> , 1998, 315, 117-122.	0.3	9
246	Theoretical studies on field-induced superconductivity in molecular crystals. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 608-618.	2.0	9
247	Utility of chemical indices for transition structures of pericyclic reactions: Case study of the cope rearrangement. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 532-545.	2.0	9
248	Theoretical studies on magnetic interaction in one-dimensional spin chains of hydrogen atoms (Hn) and copper bromide (CuBr _n). <i>International Journal of Quantum Chemistry</i> , 2004, 100, 907-917.	2.0	9
249	Possibilities of molecule-based spintorics of DNA wires, sheets, and related materials. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 655-671.	2.0	9
250	Chemical bonding, less screening, and Hund's rule revisited. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 687-700.	2.0	9
251	Theoretical studies on relation among structures, electric structures and magnetic interactions in MMX complexes. <i>Polyhedron</i> , 2007, 26, 2154-2160.	2.2	9
252	Instability in Chemical Bonds from Broken-Symmetry Single-Reference to Symmetry-Adapted Multireference Approaches to Strongly Correlated Electron Systems. , 2009, , .		9

#	ARTICLE	IF	CITATIONS
253	Does B3LYP correctly describe magnetism of manganese complexes with various oxidation numbers and various structural motifs?. <i>Chemical Physics Letters</i> , 2012, 519-520, 134-140.	2.6	9
254	Understanding Two Different Structures in the Dark Stable State of the Oxygen-Evolving Complex of Photosystem-II: Applicability of the Jahn-Teller Deformation Formula. <i>ChemPhotoChem</i> , 2018, 2, 257-270.	3.0	9
255	Theoretical studies of photo-oxidative cleavage reactions of nitrogen-activated C=C double bonds of enamines, indoles, and tryptamines. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 393-406.	2.0	8
256	Spin Glass Behavior of Synthetic Atacamite, $\text{Cu}_2\text{Cl}(\text{OH})_3$. <i>Molecular Crystals and Liquid Crystals</i> , 1995, 274, 113-118.	0.3	8
257	Theoretical Approaches to Molecular Magnetism II: No-Overlap and Orientation Principles for Ferromagnetic Interactions. <i>Molecular Crystals and Liquid Crystals</i> , 1995, 272, 117-129.	0.3	8
258	Visualization of two-body electron densities and wave functions of magnetic molecules. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 645-654.	2.0	8
259	Frequency-dependent second hyperpolarizabilities in the time-dependent restricted open-shell Hartree-Fock theory: Application to the Li, Na, K, and N atoms. <i>Journal of Chemical Physics</i> , 2000, 112, 7903-7918.	3.0	8
260	QED-SCF, MCSCF, and coupled-cluster methods in quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 272-280.	2.0	8
261	Theoretical studies of molecule-based magnetic conductors. <i>Polyhedron</i> , 2003, 22, 2077-2090.	2.2	8
262	Formulation of unrestricted and restricted Hartree-Fock-Bogoliubov equations. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 10-16.	2.0	8
263	J-model for magnetism and superconductivity of triangular, kagome, and related spin lattice systems. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1179-1196.	2.0	8
264	Theory of chemical bonds in metalloenzymes XII: Electronic and spin structures of metallo-oxo and isoelectronic species and spin crossover phenomena in oxygenation reactions. <i>Polyhedron</i> , 2009, 28, 2044-2052.	2.2	8
265	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. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5099-5104.	2.5	8
266	A resonating broken symmetry configuration interaction approach for double-exchange magnetic systems. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 064227.	1.8	8
267	Theoretical study of intra- and inter-chain magnetic interactions in $[\text{Ni}(\text{chxn})_2\text{Br}]\text{Br}_2$. <i>Polyhedron</i> , 2011, 30, 3116-3120.	2.2	8
268	Theory of chemical bonds in metalloenzymes - Manganese oxides clusters in the oxygen evolution center -. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	8
269	Linear response function approach for the boundary problem of QM/MM methods. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 336-341.	2.0	8
270	Theory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn_5O_5 , CaMn_4O_5 and $\text{Ca}_2\text{Mn}_3\text{O}_5$ clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesis. <i>Polyhedron</i> , 2013, 57, 138-149.	2.2	8

#	ARTICLE	IF	CITATIONS
271	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.	3.2	8
272	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.	2.6	8
273	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.	2.6	8
274	MOLECULAR ORBITALS OF ANTIAROMATIC MOLECULES: CYCLIC POLYMETHINES (CH) ₃ and (CH) ₄ . Chemistry Letters, 1977, 6, 971-974.	1.3	7
275	New Cation-Diffusing Phase of (CH ₃ NH ₃) ₅ Bi ₂ Cl ₁₁ . Journal of the Physical Society of Japan, 1995, 64, 391-394.	1.6	7
276	Ab Initio mo Calculations of Superexchange Integrals For Transition-Metal Fluorides: MF _M ³⁺ (M=Cu(?), Ni(II) and Mn(II)). Active Control of the Magnetic States. Molecular Crystals and Liquid Crystals, 1996, 286, 185-192.	0.3	7
277	Solid State ¹ H-Mas-Nmr and Spin Densities on Protons of the Organic Ferromagnetic Tempo Derivatives. Molecular Crystals and Liquid Crystals, 1997, 306, 307-314.	0.3	7
278	Generalized spin orbital GW theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 369-374.	2.0	7
279	Theoretical Studies on Magnetic Interactions of Aligned Tetrametal Systems by Using Magnetic Effective Density Functional (MEDF) Method. Molecular Crystals and Liquid Crystals, 2002, 379, 525-530.	0.9	7
280	Spin-orbit coupling of spin-frustrated systems. International Journal of Quantum Chemistry, 2005, 102, 80-89.	2.0	7
281	Resonating coupled-cluster CI approach to ion-radical systems: Comparison with the unrestricted coupled-cluster approach. International Journal of Quantum Chemistry, 2009, 109, 3811-3818.	2.0	7
282	Theoretical study of absorption spectrum of dirhodium tetracarboxylate complex [Rh ₂ (CH ₃ COO) ₄ (H ₂ O) ₂] in aqueous solution revisited. Supramolecular Chemistry, 2011, 23, 329-336.	1.2	7
283	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.	2.2	7
284	Theoretical Investigation on Nearsightedness of Finite Model and Molecular Systems Based on Linear Response Function Analysis. Molecules, 2014, 19, 13358-13373.	3.8	7
285	Theory of chemical bonds in metalloenzymes XX: magneto-structural correlations in the CaMn ₄ O ₅ cluster in oxygen-evolving complex of photosystem II. Molecular Physics, 2015, , 1-28.	1.7	7
286	Theory of chemical bonds in metalloenzymes XXII: a concerted bond-switching mechanism for the oxygen-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.	1.7	7
287	Relative stability among intermediate structures in S ₂ state of CaMn ₄ O ₅ 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.	3.9	7
288	Magnetic Behavior of Polymers Containing Paramagnetic Metalloporphyrins. Molecular Crystals and Liquid Crystals, 1995, 273, 117-124.	0.3	6

#	ARTICLE	IF	CITATIONS
289	Theoretical Studies of Direct Exchange Couplings Between Transition Metal Ions II. Tetranuclear Transition Metal Systems. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 286, 201-210.	0.3	6
290	Theoretical study on rotational barriers of 1,3-dipoles and mechanisms of 1,3-dipolar reactions. , 1997, 2, 218-235.		6
291	Electron correlation and structure dependencies of the second hyperpolarizability of ethylene. <i>International Journal of Quantum Chemistry</i> , 1999, 71, 177-183.	2.0	6
292	Self-consistent-field calculations of molecular magnetic properties using gauge-invariant atomic orbitals. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 637-643.	2.0	6
293	Theoretical study on dependency of conductivity on structure of the proton- and electron-coupled system. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 882-891.	2.0	6
294	Theoretical Study on Necessary Conditions for Reversible Photoinduced Magnetization: Cobalt-Iron Cyanide System. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 343, 151-156.	0.3	6
295	Theoretical Studies on Radical Spin Arrangements in the Cavity of Nanoporous Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 343, 215-220.	0.3	6
296	Ab Initio Molecular Orbital Study on Thermal and Photochemical Reactions of 3-Furyl, 3-Pyrryl, and 3-Thienyl Fulgies. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 345, 81-88.	0.3	6
297	Intermolecular-interaction effects on quantum-phase dynamics of dimer systems interacting with a two-mode squeezed vacuum field. <i>Journal of Chemical Physics</i> , 2002, 117, 9671-9687.	3.0	6
298	Theoretical studies on magnetic interactions between Ni(II) ions in urease. <i>Polyhedron</i> , 2005, 24, 2778-2783.	2.2	6
299	Theory of chemical bonds in metalloenzymes XI: Full geometry optimization and vibration analysis of porphyrin iron-oxo species. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2950-2965.	2.0	6
300	Locality and nonlocality of electronic structures of molecular systems: Toward QM/MM and QM/QM approaches. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	6
301	Comparison of Effective Exchange Integrals of H-H and H-He-H Chains vs. Single Molecules: A Theoretical Study. <i>Chemistry Letters</i> , 2020, 49, 137-140.	1.3	6
302	Instability of the restricted Hartree-Fock (RHF) solution for the triplet state. <i>Molecular Physics</i> , 1978, 35, 33-49.	1.7	5
303	Theoretical Studies of Direct Exchange Couplings Between Transition Metal Ions I. Naked Binuclear Chromium(II) and Molybdenum (II) Systems. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 286, 193-200.	0.3	5
304	Theoretical Studies on Magnetic Interaction of Di- μ -oxo Bridged Manganese Dimers. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 343, 157-162.	0.3	5
305	Monte Carlo wave-function approach to the quantum-phase dynamics of a dissipative molecular system interacting with a single-mode amplitude-squeezed field. <i>Journal of Chemical Physics</i> , 2003, 119, 12106-12118.	3.0	5
306	Search for the ground states of Ising spin clusters by using the genetic algorithms. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 645-654.	2.0	5

#	ARTICLE	IF	CITATIONS
307	Spin-optimized resonating Hartree-Fock configuration interaction. International Journal of Quantum Chemistry, 2007, 107, 3219-3227.	2.0	5
308	Estimation of effective exchange integral value of polyradical systems based on the band calculation. International Journal of Quantum Chemistry, 2009, 109, 3632-3640.	2.0	5
309	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.	2.8	5
310	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.	1.7	5
311	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.	2.6	5
312	Heisenberg model for radical reactions. Part 3. Direct exchange coupling between transition metal ions and triplet methylene. Computational and Theoretical Chemistry, 1994, 310, 185-196.	1.5	4
313	π-Conjugated Polyradicals With Poly(Phenylene-Vinylene) Skeleton and Their Through-Bond and Long-Range Interaction. Molecular Crystals and Liquid Crystals, 1995, 272, 131-138.	0.3	4
314	Nonadiabatic treatment of molecular systems by the wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1261-1270.	2.0	4
315	Calculation of Magnetization by Path Integral Method II. Molecular Crystals and Liquid Crystals, 1996, 286, 177-184.	0.3	4
316	Calculation of Magnetization by Path Integral Method I. Molecular Crystals and Liquid Crystals, 1996, 286, 171-176.	0.3	4
317	Theoretical Studies of Magnetic Interactions in <i>p</i> -Cyanophenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1997, 306, 331-338.	0.3	4
318	Casscf Calculations for Neutral and Anion Radical States of Several π-Conjugated Bis-Methylene Systems. Molecular Crystals and Liquid Crystals, 1997, 306, 475-486.	0.3	4
319	Theoretical Studies of one Dimensional Tetranuclear Transition Metal Systems and their Clusters. Molecular Crystals and Liquid Crystals, 1997, 306, 463-474.	0.3	4
320	Theoretical studies on magnetic behavior in clusters by the genetic algorithms. International Journal of Quantum Chemistry, 2000, 80, 646-656.	2.0	4
321	Variable Magnetism of Layer-Structured Compounds Cu2(OD)3X with Exchangeable Anion X: Magnetic Local Structure and Magnetic Interactions Determined by Solid-State High-Resolution Deuterium NMR. Molecular Crystals and Liquid Crystals, 2000, 341, 369-376.	0.3	4
322	Theoretical Studies on Magnetic Interactions of Dichromium Tetraacetate by Using Hybrid Density Functional Method. Molecular Crystals and Liquid Crystals, 2000, 343, 145-150.	0.3	4
323	Analysis of difference two-electron density matrix between two states of magnetic molecules. International Journal of Quantum Chemistry, 2001, 85, 204-213.	2.0	4
324	Theoretical Studies on the Electronic States of Hole-Doped Copper Oxides. Molecular Crystals and Liquid Crystals, 2002, 379, 507-512.	0.9	4

#	ARTICLE	IF	CITATIONS
325	Theoretical Study on the Magnetic Interaction for Manganese Oxides. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 376, 335-340.	0.9	4
326	Quantum electrodynamical density-matrix functional theory and group theoretical consideration of its solution. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 273-281.	2.0	4
327	One- and two-exciton migration dynamics of a dendritic molecular aggregate. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 472-478.	2.0	4
328	THEORETICAL STUDY ON THE SECOND HYPERPOLARIZABILITY ($\hat{\chi}^3$) OF A HOMOGENEOUS MOLECULE IN THE BOND DISSOCIATION PROCESS: ENHANCEMENT OF $\hat{\chi}^3$ IN THE INTERMEDIATE CORRELATION REGIME. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2004, 13, 411-416.	1.8	4
329	N-band Hubbard models. III. Boson-fermion and interaction-boson models for high-Tc superconductivity. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1052-1075.	2.0	4
330	The electronic structure and magnetic property of $\hat{1}/4$ -hydroxo bridged manganese porphyrin dimer. <i>European Physical Journal D</i> , 2006, 38, 193-197.	1.3	4
331	Many-electron-wavepackets method. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1291-1301.	2.0	3
332	Theoretical study on electronic structures of oxygenated dipoles and mechanisms of ozonolysis reactions. , 1997, 2, 236-252.		3
333	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 697-707.	2.0	3
334	Theoretical Studies of the Pressure Effects for $\hat{1}/2$ -Phase of p-NPNN. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 623-632.	0.3	3
335	Numerical coupled Liouville approach: Application to second hyperpolarizability of molecular aggregate. <i>International Journal of Quantum Chemistry</i> , 1999, 71, 295-306.	2.0	3
336	Ab Initio Crystal Orbital Study of Ferromagnetic Interactions of Spins in Polymer Comprising Phenylenevinylene. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 613-622.	0.3	3
337	Dynamics of Magnetization for a System ($S=3$) with Strong Uniaxial Magnetocrystalline Anisotropy. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 593-602.	0.3	3
338	Magic Angle Spinning $^1\text{H-NMR}$ Study of the Spin Density Distribution of Pyridyl Nitronyl Nitroxides in the Crystalline Phase. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 334, 295-304.	0.3	3
339	Generalized Spin-Density Functional Calculation for the Spin Frustrated Systems. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 343, 139-144.	0.3	3
340	Molecular Simulations of Argon, Nitrogen, and Hydrogen Adsorption in Microporous Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 285-290.	0.3	3
341	Third-order nonlinear optical properties of dendritic molecular aggregates: Effects of fractal architecture. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 649-659.	2.0	3
342	Theoretical Studies with C_{60} Cluster Models for Pure Organomagnetic Conductors. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 483-488.	0.9	3

#	ARTICLE	IF	CITATIONS
343	Monte Carlo Wave Function (MCWF) approach to dissipative quantum systems interacting with a single-mode quantized field. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 461-471.	2.0	3
344	Ab initio study for static hyperpolarizabilities of several donor-acceptor molecules. <i>Molecular Physics</i> , 2003, 101, 309-314.	1.7	3
345	Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 927-936.	2.0	3
346	The Nature of Effective Exchange Interactions. , 2006, , 201-228.		3
347	Theoretical study of magnetic interaction between C60 anion radicals. <i>Polyhedron</i> , 2009, 28, 1750-1753.	2.2	3
348	Theoretical studies on the structural and magnetic property of arginase active site. <i>Supramolecular Chemistry</i> , 2011, 23, 22-28.	1.2	3
349	Linear Response Functions of Densities and Spin Densities for Systematic Modeling of the QM/MM Approach for Mono- and Poly-Nuclear Transition Metal Systems. <i>Molecules</i> , 2019, 24, 821.	3.8	3
350	Domain-based local pair natural orbital CCSD(T) calculations of strongly correlated electron systems: Examination of dynamic equilibrium models based on multiple intermediates in S ₁ state of photosystem II. <i>Molecular Physics</i> , 2020, 118, e1666171.	1.7	3
351	Development of broken-symmetry (BS) methods in chemical reactions. A theoretical view of water oxidation in photosystem II and related systems. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 402, 112791.	3.9	3
352	A three states model for hydrogen abstraction reactions with the cytochrome P450 compound I is revisited. Isolobal and isospin analogy among Fe(IV)=O, O ⁻ =O and O. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 405, 112902.	3.9	3
353	Density functional theory without the Born-Oppenheimer approximation and its application. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 659-669.	2.0	3
354	Generalized spin density functional theory for noncollinear molecular magnetism. , 2000, 80, 664.		3
355	Theoretical Studies of Spin Populations on Nitronyl Nitroxide, Phenyl Nitronyl Nitroxide and P-NPNN. <i>Molecular Crystals and Liquid Crystals</i> , 1995, 271, 19-28.	0.3	2
356	Magnetic Properties of Polymers Containing Paramagnetic Metalloporphyrins in Their Main Chain. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 25-32.	0.3	2
357	Theoretical Studies of Intra- and Inter- Magnetic Interactions in TMAO(1,3,5,7 - Tetramethyl - 2, 6-) Tj ETQq1 1 0.784314 rgBT ₂ /Overlo	0.3	2
358	Quantum Phase Dynamics of Interaction between Photon Field and Magnetic System: Effects of Magnetic Quantum Tunnelling. <i>Optical Review</i> , 1999, 6, 227-231.	2.0	2
359	Third-Order Nonlinear Optical Properties of π -Conjugated Systems Involving Sulfur Atoms: A Proposal of Multi-Property Materials Combining Conductivity and Unique Third-Order Nonlinearity. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 337, 369-372.	0.3	2
360	Exciton Condensate in Model Dendrimers. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 273-278.	0.3	2

#	ARTICLE	IF	CITATIONS
361	Exciton Migration Dynamics of D58-like Dendritic Molecular Aggregate. <i>Molecular Crystals and Liquid Crystals</i> , 2001, 371, 345-348.	0.3	2
362	Generalized Spin Orbital Density Functional Study of Multicenter Metal Systems. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 537-542.	0.9	2
363	Theoretical Study on Open-Shell Nonlinear Optical Systems. <i>Materials Research Society Symposia Proceedings</i> , 2004, 846, DD1.4.1.	0.1	2
364	Quantum-phase dynamics of molecular systems interacting with a two-mode squeezed vacuum field: Detuning effects. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 421-430.	2.0	2
365	Fractional occupation number approaches for CAS (2,2) systems based on second-order density. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 658-665.	2.0	2
366	Theoretical studies on the electronic structure of the synthetic complex of soluble methanemonooxygenase intermediate Q. <i>Supramolecular Chemistry</i> , 2011, 23, 83-87.	1.2	2
367	Nearsightedness-related indices of finite systems based on linear response function: one-dimensional cases. <i>Molecular Physics</i> , 0, , 1-9.	1.7	2
368	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. <i>Molecular Physics</i> , 2017, 115, 2154-2167.	1.7	2
369	UNO(ULO) active space for multireference calculations on classical and quantum computers. Revisit to the iron-sulfur complexes. <i>Chemical Physics Letters</i> , 2020, 746, 137252.	2.6	2
370	Theory of chemical bonds in metalloenzymes XXIII fundamental principles for the photo-induced water oxidation in oxygen evolving complex of photosystem II. <i>Molecular Physics</i> , 2020, 118, e1725168.	1.7	2
371	Polarizabilities and Hyperpolarizabilities of Dendritic Systems. <i>Advances in Multi-photon Processes and Spectroscopy</i> , 2003, , 3-146.	0.6	2
372	Theoretical Studies on Nonlinear Optical Properties of Organometallic Conjugated Systems I: Static Third-Order Hyperpolarizabilities of First- Transition-Metal and Metal-Methylene Cations. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 286, 159-164.	0.3	1
373	Magnetic Properties Of Basic Copper(?) Formates. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 286, 17-22.	0.3	1
374	Theoretical Study and Comparison with Experiments for Atacamite, $\text{Cu}_2\text{Cl}(\text{OH})_3$. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 33-40.	0.3	1
375	Numerical Coupled Liouville Approach: Dependence of Polarizability on Field Intensity and the Size of Linear Molecular Aggregates. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6807-6811.	2.5	1
376	Theoretical Studies of Magnetic Interactions in Cu^{2+} , Ni^{2+} -Dihydroxyphenyl Nitronyl Nitroxide Crystal. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 633-642.	0.3	1
377	Theoretical Studies on the Second Hyperpolarizabilities of Trithiapentalene and Its Donor and Acceptor Disubstituted Species. <i>Optical Review</i> , 1999, 6, 232-236.	2.0	1
378	Quantum-phase and information-entropy dynamics of dimers interacting with a single-mode coherent field: The difference between one- and two-exciton models. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 530-545.	2.0	1

#	ARTICLE	IF	CITATIONS
379	Electronic structure calculation by monte carlo diagonalization method. International Journal of Quantum Chemistry, 2001, 84, 601-606.	2.0	1
380	Theoretical Studies on Magnetic Interactions of Aligned Tetrametal System by Using Hybrid Density Functional Method. Molecular Crystals and Liquid Crystals, 2002, 376, 347-352.	0.9	1
381	Theoretical Studies on Magnetic Couplings of M- π Conjugated Systems via Pyrimidine Coupler. Molecular Crystals and Liquid Crystals, 2002, 379, 531-536.	0.9	1
382	Theoretical Studies on π -d Magnetic Interactions Between BETS Donor and Transition Metal Halides in π -BETS 2 MX 4 Crystals. Molecular Crystals and Liquid Crystals, 2002, 379, 489-494.	0.9	1
383	Theoretical studies on dissociation of metal-carbon bond in Cobalamin: Formulation and calculation. Polyhedron, 2005, 24, 2745-2750.	2.2	1
384	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. Molecular Crystals and Liquid Crystals, 2006, 455, 135-141.	0.9	1
385	Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order Møller-Plesset perturbation theory level based on the quasi-energy derivative method. , 1997, 65, 665.		1
386	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. , 1997, 65, 697.		1
387	Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order Møller-Plesset perturbation theory level based on the quasi-energy derivative method. International Journal of Quantum Chemistry, 1997, 65, 665-677.	2.0	1
388	Hyperpolarizabilities of one-dimensional H_n systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. International Journal of Quantum Chemistry, 1998, 70, 269-282.	2.0	1
389	Density functional theory without the Born-Oppenheimer approximation. II. Green function techniques. , 1999, 75, 875.		1
390	Theoretical study on dependency of conductivity on structure of the proton- and electron-coupled system. , 2000, 80, 882.		1
391	A novel inclusion complex between molybdenum(II) fumarate and poly(ethylene glycol): first supramolecule formation between a microporous complex and an organic polymer. , 2000, 11, 840.		1
392	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
393	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
394	Isolobal and isospin analogy between organic and inorganic open-shell molecules 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.	0.8	1
395	Theoretical studies on hyperpolarizabilities of nitroxide species I. , 1994, , .		0
396	ESR and NMR study on the charge-transfer complexes of N-Salicylideneanilines containing NHO hydrogen bond as a dynamic function. , 1994, , .		0

#	ARTICLE	IF	CITATIONS
397	Molecular Structure And Magnetic Characterization Of Structurally Reinforced Chiral Macrocyclic Poly- Amine-Based Dinuclear Copper(II) Complexes by x- and w- band ESR Spectroscopy and Squid Measurements. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 286, 43-50.	0.3	0
398	Casci and Casscf Studies of Dinuclear Transition Metal Systems with Quadruple Metal-Metal Bonds (M=Cr(Ii), Mo(Ii)). <i>Molecular Crystals and Liquid Crystals</i> , 1997, 306, 321-330.	0.3	0
399	Theoretical Studies on Hyperpolarizabelities of Nitroxide Species II. Second Hyperpolarizability of p-NPNN. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 294, 251-254.	0.3	0
400	Three Dimensional Wavepacket Simulation on the H Atom Scattering for the Full Reaction of $CF_3 + Ar \rightarrow CF_3 + H + Ar$. <i>Israel Journal of Chemistry</i> , 1997, 37, 359-365.	2.3	0
401	Numerical coupled Liouville approach: Quantum dynamics of linear molecular aggregates under intense electric fields. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 77-87.	2.0	0
402	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 337, 393-396.	0.3	0
403	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. <i>Optical Review</i> , 1999, 6, 237-241.	2.0	0
404	Polarizabilities of Dendritic Molecular Aggregates: Contribution of Exciton Generation. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 303-308.	0.3	0
405	Theoretical Study on Magnetic Interactions of Mn- π Conjugated System. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 291-296.	0.3	0
406	Theoretical Studies on Quantum Tunneling of Spins in Cluster of Clusters. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 279-284.	0.3	0
407	Exciton Migration Pathways in Dendritic Molecular Aggregates. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 342, 297-302.	0.3	0
408	Theoretical Study on Near-Resonant Third-Order Nonlinear Optical Properties ($\hat{\chi}^3$) of Dendritic Molecular Aggregates: Intermolecular-Interaction and Relaxation Effects on $\hat{\chi}^3$. <i>Molecular Crystals and Liquid Crystals</i> , 2001, 371, 261-264.	0.3	0
409	Theoretical study on quantum dynamics of bose system interacting with photon field. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 401-408.	2.0	0
410	Three-dimensional multi-layered optical memory using dye and Au(III) doped SiO ₂ /TiO ₂ sol-gel medium. , 0, , .		0
411	Theoretical Study on the Polarizabilities of Two-Dimensionally-Grown Dendritic Molecular Aggregates: The Artichitecture- and Size-Dependency. <i>Molecular Crystals and Liquid Crystals</i> , 2001, 371, 215-218.	0.3	0
412	NONLINEAR OPTICAL PROPERTIES OF SEVERAL π -CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. <i>International Journal of Nanoscience</i> , 2002, 01, 651-655.	0.7	0
413	THEORETICAL STUDY OF EXCITON-EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. <i>International Journal of Nanoscience</i> , 2002, 01, 713-717.	0.7	0
414	Field-induced Superconductivity. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 495-500.	0.9	0

#	ARTICLE	IF	CITATIONS
415	Estimation of Transfer Matrix of AgO System. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 519-524.	0.9	0
416	Molecular Dynamics Simulation of Metal Oxides Including Ag. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 501-506.	0.9	0
417	Theoretical Studies on SDW and CDW States of Cu and Ag Oxides under the Periodic Boundary Condition. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 379, 513-518.	0.9	0
418	Theoretical Studies on Magnetic Properties of TCNQ Organic Crystals with Ab initio and DFT Methods. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 376, 411-416.	0.9	0
419	AB INITIO STUDY ON NONLINEAR OPTICAL PROPERTIES FOR SMALL DENDRITIC MOLECULES. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2004, 13, 417-422.	1.8	0
420	Determination of the Hubbard model parameters by using the unrestricted Hartree-Fock solutions, and improvement of their energies. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 73-81.	2.0	0
421	Derivation of dynamic electric and magnetic response properties based on the quasienergy derivative method. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2007, 6, 397-427.	0.2	0
422	N ^d bands Hubbard models. IV. Comparisons of electron ^d -or hole ^d -doped quaternary oxypictides LaOMPn superconductors with cuprates. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 3016-3041.	2.0	0
423	Reprint of ^d Theory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn ₅ O ₅ , CaMn ₄ O ₅ and Ca ₂ Mn ₃ O ₅ clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesis ^d . <i>Polyhedron</i> , 2013, 66, 283-293.	2.2	0
424	Electronic Structure of the CaMn ₄ O ₅ Cluster in the PSII System Refined to the 1.9 Å... X-ray Resolution. Possible Mechanisms of Photosynthetic Water Splitting. <i>Advanced Topics in Science and Technology in China</i> , 2013, , 250-254.	0.1	0
425	First principle calculations of effective exchange integrals: Comparison between SR (BS) and MR computational results. , 2015, , .		0
426	Development of approximate spin projection method and its application for elucidation of electronic structures, molecular structures and physical properties of polynuclear metal complexes. <i>Bulletin of Japan Society of Coordination Chemistry</i> , 2018, 71, 57-68.	0.2	0
427	Mechanism of Water Oxidation in Photosynthesis Elucidated by Interplay Between Experiment and Theory. <i>Advances in Photosynthesis and Respiration</i> , 2021, , 39-80.	1.0	0
428	SECOND HYPERPOLARIZABILITIES OF MOLECULAR AGGREGATES: INTERMOLECULAR ORBITAL-INTERACTION AND SPIN-CONFIGURATION EFFECTS. , 2003, , .		0
429	THEORETICAL STUDY OF EXCITON ^d EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. , 2003, , .		0
430	NONLINEAR OPTICAL PROPERTIES OF SEVERAL ^d -CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. , 2003, , .		0
431	CHARGE-TRANSFER-INDUCED LUMINESCENCE (CTIL) MECHANISMS OF CHEMI- AND BIOLUMINESCENCE REACTIONS. , 2008, , .		0
432	THEORETICAL CONSIDERATIONS ON THE ROLES OF HYDROGEN BONDING IN THERMAL DECOMPOSITION OF PEROXIDES. , 2008, , .		0

#	ARTICLE	IF	CITATIONS
433	The Reaction Mechanisms of O ₂ Formation in Photosynthesis. Seibutsu Butsuri, 2018, 58, 127-133.	0.1	0