Kizashi Yamaguchi

List of Publications by Year
in descending order

433	12,834	34076	38368
papers	citations	52 h-index	95 g-index

433	433	433	5952
all docs	docs citations	times ranked	citing authors

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

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

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

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

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

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

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

#	Article	IF	Citations
127	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Feï£¿2S] clusters. International Journal of Quantum Chemistry, 2007, 107, 609-627.	1.0	32
128	Ab initio calculation of the Dzyaloshinskiiâ€“Moriya parameters: Spinâ€“orbit GSO-HF, DFT, and CI approaches. International Journal of Quantum Chemistry, 2007, 107, 1328-1334.	1.0	16
129	Density functional study of manganese dimer. International Journal of Quantum Chemistry, 2007, 107, 3178-3190.	1.0	21
130	Geometry optimization method based on approximate spin projection and its application to F₂, CH₂, CH₂OO, and active site of urease. International Journal of Quantum Chemistry, 2007, 107, 3094-3102.	1.0	24
131	Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase and the related species. International Journal of Quantum Chemistry, 2007, 107, 3250-3265.	1.0	13
132	Spinâ€optimized resonating Hartreeâ€Fock configuration interaction. International Journal of Quantum Chemistry, 2007, 107, 3219-3227.	1.0	5
133	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. Molecular Crystals and Liquid Crystals, 2006, 455, 135-141.	0.4	1
134	Recent Development of Multireference Density Functional Theory. Chemistry Letters, 2006, 35, 242-247.	0.7	25
135	The Nature of Effective Exchange Interactions. , 2006, , 201-228.		3
136	N-band Hubbard models. III. Boson-fermion and interaction-boson models for high-Tcsuperconductivity. International Journal of Quantum Chemistry, 2006, 106, 1052-1075.	1.0	4
137	CASSCF version of density functional theory. International Journal of Quantum Chemistry, 2006, 106, 3325-3333.	1.0	18
138	Multireference density functional theory with orbital-dependent correlation corrections. International Journal of Quantum Chemistry, 2006, 106, 3312-3324.	1.0	33
139	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Feâ€“7S] core. International Journal of Quantum Chemistry, 2006, 106, 3288-3302.	1.0	28
140	Resonating broken-symmetry approach to biradicals and polyradicals. International Journal of Quantum Chemistry, 2006, 106, 3303-3311.	1.0	20
141	Hybrid-density functional study of magnetism and ligand control in Ni9 complexes. Chemical Physics Letters, 2006, 421, 483-487.	1.2	19
142	A general algorithm for calculation of Heisenberg exchange integrals J in multispin systems. Chemical Physics Letters, 2006, 432, 343-347.	1.2	268
143	The electronic structure and magnetic property of Î¼-hydroxo bridged manganese porphyrin dimer. European Physical Journal D, 2006, 38, 193-197.	0.6	4
144	Theoretical studies on dissociation of metalâ€“carbon bond in Cobalamin: Formulation and calculation. Polyhedron, 2005, 24, 2745-2750.	1.0	1

#	Article	IF	Citations
145	Theoretical studies on magnetic interactions and charge-dope effects in one-dimensional Ni5 and Ni7 complexes. Polyhedron, 2005, 24, 2751-2757.	1.0	15
146	Theoretical studies on ferrimagnetic behavior of TCNE and manganese porphyrin dimer. Polyhedron, 2005, 24, 2720-2725.	1.0	14
147	Theoretical study on the magnetic interactions of active site in hemerythrin. Polyhedron, 2005, 24, 2701-2707.	1.0	14
148	Theoretical studies on magnetic interactions between Ni(II) ions in urease. Polyhedron, 2005, 24, 2778-2783.	1.0	6
149	Electronic and spin structures of manganese clusters in the photosynthesis II system. Polyhedron, 2005, 24, 2767-2777.	1.0	58
150	Fractional occupation number approaches for CAS (2,2) systems based on second-order density. International Journal of Quantum Chemistry, 2005, 101, 658-665.	1.0	2
151	Spin-orbit coupling of spin-frustrated systems. International Journal of Quantum Chemistry, 2005, 102, 80-89.	1.0	7
152	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of ?-conjugated oligomers by intermolecular interaction. International Journal of Quantum Chemistry, 2005, 102, 702-710.	1.0	20
153	Determination of the Hubbard model parameters by using the unrestricted Hartree-Fock solutions, and improvement of their energies. International Journal of Quantum Chemistry, 2005, 103, 73-81.	1.0	0
154	Search for the ground states of Ising spin clusters by using the genetic algorithms. International Journal of Quantum Chemistry, 2005, 105, 645-654.	1.0	5
155	Quantum spin correction scheme for ab initio spin-unrestricted solutions: Multiple bonds case. International Journal of Quantum Chemistry, 2005, 105, 605-614.	1.0	26
156	Possibilities of molecule-based spintoronics of DNA wires, sheets, and related materials. International Journal of Quantum Chemistry, 2005, 105, 655-671.	1.0	9
157	Chemical bonding, less screening, and Hund's rule revisited. International Journal of Quantum Chemistry, 2005, 105, 687-700.	1.0	9
158	Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. International Journal of Quantum Chemistry, 2005, 105, 615-627.	1.0	11
159	Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron-sulfur clusters. International Journal of Quantum Chemistry, 2005, 105, 628-644.	1.0	25
160	Theoretical Study on Open-Shell Nonlinear Optical Systems. Materials Research Society Symposia Proceedings, 2004, 846, DD1.4.1.	0.1	2
161	AB INITIO STUDY ON NONLINEAR OPTICAL PROPERTIES FOR SMALL DENDRITIC MOLECULES. Journal of Nonlinear Optical Physics and Materials, 2004, 13, 417-422.	1.1	0
162	THEORETICAL STUDY ON THE SECOND HYPERPOLARIZABILITY (Î³) OF A HOMOGENEOUS MOLECULE IN THE BOND DISSOCIATION PROCESS: ENHANCEMENT OF Î³ IN THE INTERMEDIATE CORRELATION REGIME. Journal of Nonlinear Optical Physics and Materials, 2004, 13, 411-416.	1.1	4

#	Article	IF	Citations
163	Formulation of unrestricted and restricted Hartree-Fock-Bogoliubov equations. International Journal of Quantum Chemistry, 2004, 96, 10-16.	1.0	8
164	Approximate on-top pair density into one-body functions for CAS-DFT. International Journal of Quantum Chemistry, 2004, 96, 463-473.	1.0	28
165	Quantum-phase dynamics of molecular systems interacting with a two-mode squeezed vacuum field: Detuning effects. International Journal of Quantum Chemistry, 2004, 99, 421-430.	1.0	2
166	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.	1.0	42
167	Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. International Journal of Quantum Chemistry, 2004, 100, 927-936.	1.0	3
168	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.	1.0	49
169	Theoretical studies on magnetic interaction in one-dimensional spin chains of hydrogen atoms (Hn) and copper bromide (CunBrm). International Journal of Quantum Chemistry, 2004, 100, 907-917.	1.0	9
170	J-model for magnetism and superconductivity of triangular, kagome, and related spin lattice systems. International Journal of Quantum Chemistry, 2004, 100, 1179-1196.	1.0	8
171	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.	2.0	26
172	Density functional study of tetrahedral manganese clusters. Polyhedron, 2003, 22, 2013-2017.	1.0	31
173	Hybrid DFT study of electronic structure on quasi-one-dimensional halogen-bridged binuclear metal complexes (MMX). Polyhedron, 2003, 22, 2027-2038.	1.0	20
174	Theoretical studies of molecule-based magnetic conductors. Polyhedron, 2003, 22, 2077-2090.	1.0	8
175	Fractional occupation numbers and spin density functional calculations of degenerate systems. International Journal of Quantum Chemistry, 2003, 93, 317-323.	1.0	11
176	Generalized spin density functional study of radical reactions. International Journal of Quantum Chemistry, 2003, 91, 376-383.	1.0	18
177	N-band Hubbard models II: Cooperative mechanisms of electron-phonon, electron correlation, and many-band effects toward high-Tc superconductors. International Journal of Quantum Chemistry, 2003, 92, 47-70.	1.0	11
178	One- and two-exciton migration dynamics of a dendritic molecular aggregate. International Journal of Quantum Chemistry, 2003, 95, 472-478.	1.0	4
179	Monte Carlo Wave Function (MCWF) approach to dissipative quantum systems interacting with a single-mode quantized field. International Journal of Quantum Chemistry, 2003, 95, 461-471.	1.0	3
180	Spin correlation functions by generalized spin orbital density functional and multireference approaches. International Journal of Quantum Chemistry, 2003, 95, 512-520.	1.0	16

#	Article	IF	Citations
181	Utility of chemical indices for transition structures of pericyclic reactions: Case study of the cope rearrangement. International Journal of Quantum Chemistry, 2003, 95, 532-545.	1.0	9
182	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.	1.9	41
183	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.	1.2	27
184	Monte Carlo wave-function approach to the quantum-phase dynamics of a dissipative molecular system interacting with a single-mode amplitude-squeezed field. Journal of Chemical Physics, 2003, 119, 12106-12118.	1.2	5
185	Ab initiostudy for static hyperpolarizabilities of several donor-Ï€-acceptor molecules. Molecular Physics, 2003, 101, 309-314.	0.8	3
186	Polarizabilities and Hyperpolarizabilities of Dendritic Systems. Advances in Multi-photon Processes and Spectroscopy, 2003, , 3-146.	0.6	2
187	SECOND HYPERPOLARIZABILITIES OF MOLECULAR AGGREGATES: INTERMOLECULAR ORBITAL-INTERACTION AND SPIN-CONFIGURATION EFFECTS. , 2003, , .		0
188	THEORETICAL STUDY OF EXCITONâ€“EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. , 2003, , .		0
189	NONLINEAR OPTICAL PROPERTIES OF SEVERAL Ï€-CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. , 2003, , .		0
190	Intermolecular-interaction effects on quantum-phase dynamics of dimer systems interacting with a two-mode squeezed vacuum field. Journal of Chemical Physics, 2002, 117, 9671-9687.	1.2	6
191	Theoretical Studies on Magnetic Interactions of Aligned Tetrametal System by Using Hybrid Density Functional Method. Molecular Crystals and Liquid Crystals, 2002, 376, 347-352.	0.4	1
192	MULTIBAND SUPERCONDUCTIVITY. International Journal of Modern Physics B, 2002, 16, 3419-3428.	1.0	17
193	NONLINEAR OPTICAL PROPERTIES OF SEVERAL Ï€-CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. International Journal of Nanoscience, 2002, 01, 651-655.	0.4	0
194	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.	0.4	7
195	THEORETICAL STUDY OF EXCITONâ€“EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. International Journal of Nanoscience, 2002, 01, 713-717.	0.4	0
196	Field-induced Superconductivity. Molecular Crystals and Liquid Crystals, 2002, 379, 495-500.	0.4	0
197	Estimation of Transfer Matrix of AgO System. Molecular Crystals and Liquid Crystals, 2002, 379, 519-524.	0.4	0
198	Theoretical Studies with Ï€-Râ€¢ Cluster Models for Pure Organomagnetic Conductors. Molecular Crystals and Liquid Crystals, 2002, 379, 483-488.	0.4	3

#	Article	IF	Citations
199	Theoretical Studies on Magnetic Couplings of M-Ï€ Conjugated Systems via Pyrimidine Coupler. Molecular Crystals and Liquid Crystals, 2002, 379, 531-536.	0.4	1
200	Molecular Dynamics Simulation of Metal Oxides Including Ag. Molecular Crystals and Liquid Crystals, 2002, 379, 501-506.	0.4	0
201	Theoretical Studies on the Electronic States of Hole-Doped Copper Oxides. Molecular Crystals and Liquid Crystals, 2002, 379, 507-512.	0.4	4
202	Theoretical Studies on Ï€- d Magnetic Interactions Between BETS Donor and Transition Metal Halides in Î²-BETS 2 MX 4 Crystals. Molecular Crystals and Liquid Crystals, 2002, 379, 489-494.	0.4	1
203	Theoretical Studies on SDW and CDW States of Cu and Ag Oxides under the Periodic Boundary Condition. Molecular Crystals and Liquid Crystals, 2002, 379, 513-518.	0.4	0
204	Theoretical investigation of magnetic parameters in two-dimensional sheets of pure organic BEDT-TTF and BETS molecules by usingab initioMO and DFT methods. Molecular Physics, 2002, 100, 2641-2652.	0.8	14
205	Quantum-phase dynamics of dimer systems interacting with a two-mode squeezed coherent field. Journal of Chemical Physics, 2002, 116, 10069-10082.	1.2	11
206	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.	0.8	68
207	Theoretical Study on the Magnetic Interaction for Manganese Oxides. Molecular Crystals and Liquid Crystals, 2002, 376, 335-340.	0.4	4
208	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.	0.8	26
209	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
210	Theoretical Studies on Magnetic Properties of TCNQ Organic Crystals with Ab initio and DFT Methods. Molecular Crystals and Liquid Crystals, 2002, 376, 411-416.	0.4	0
211	Generalized Spin Orbital Density Functional Study of Multicenter Metal Systems. Molecular Crystals and Liquid Crystals, 2002, 379, 537-542.	0.4	2
212	Quantum electrodynamical density-matrix functional theory and group theoretical consideration of its solution. International Journal of Quantum Chemistry, 2002, 90, 273-281.	1.0	4
213	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.	1.0	122
214	Spin-mediated superconductivity in cuprates, organic conductors and Ï€â€“d conjugated systems. Coordination Chemistry Reviews, 2002, 226, 235-249.	9.5	24
215	CAS-DFT based on odd-electron density and radical density. Chemical Physics Letters, 2002, 366, 321-328.	1.2	56
216	Theoretical Study on Near-Resonant Third-Order Nonlinear Optical Properties (Î³) of Dendritic Molecular Aggregates: Intermolecular-Interaction and Relaxation Effects on Î³. Molecular Crystals and Liquid Crystals, 2001, 371, 261-264.	0.3	0

#	Article	IF	Citations
217	Theoretical investigation on the magnetic interaction of the tetrathiafulvaleneâ€“nitronyl nitroxide stacking model: possibility of organic magnetic metals and magnetic superconductors. Polyhedron, 2001, 20, 1169-1176.	1.0	19
218	Theoretical study of the magnetic interaction for Mâ€“Oâ€“M type metal oxides. Comparison of broken-symmetry approaches. Polyhedron, 2001, 20, 1177-1184.	1.0	60
219	6-Oxophenalenoxyl derivatives covalently linked to TTF moieties: synthesis, ESR/ENDOR measurements, and DFT calculations. Tetrahedron Letters, 2001, 42, 7991-7995.	0.7	22
220	Analysis of difference two-electron density matrix between two states of magnetic molecules. International Journal of Quantum Chemistry, 2001, 85, 204-213.	1.0	4
221	QED-SCF, MCSCF, and coupled-cluster methods in quantum chemistry. International Journal of Quantum Chemistry, 2001, 85, 272-280.	1.0	8
222	Generalized spin orbital GW theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 369-374.	1.0	7
223	Theoretical study on quantum dynamics of bose system interacting with photon field. International Journal of Quantum Chemistry, 2001, 84, 401-408.	1.0	0
224	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.	1.0	37
225	Quantum-phase and information-entropy dynamics of dimers interacting with a single-mode coherent field: The difference between one- and two-exciton models. International Journal of Quantum Chemistry, 2001, 84, 530-545.	1.0	1
226	Generalized spin orbital calculations of spin-frustrated molecules. International Journal of Quantum Chemistry, 2001, 84, 546-551.	1.0	14
227	Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. International Journal of Quantum Chemistry, 2001, 84, 592-600.	1.0	36
228	Electronic structure calculation by monte carlo diagonalization method. International Journal of Quantum Chemistry, 2001, 84, 601-606.	1.0	1
229	Third-order nonlinear optical properties of dendritic molecular aggregates: Effects of fractal architecture. International Journal of Quantum Chemistry, 2001, 84, 649-659.	1.0	3
230	Noncollinear spin density functional theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 670-676.	1.0	20
231	Theoretical studies on field-induced superconductivity in molecular crystals. International Journal of Quantum Chemistry, 2001, 85, 608-618.	1.0	9
232	Possibilities of molecular magnetic metals and highTc superconductors in field effect transistor configurations. International Journal of Quantum Chemistry, 2001, 85, 619-635.	1.0	10
233	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.	1.0	20
234	Theoretical studies on the magnetic interaction and reversible dioxygen binding of the active site in hemocyanin. Chemical Physics Letters, 2001, 335, 395-403.	1.2	38

#	Article	IF	Citations
235	Exciton Migration Dynamics of D58-like Dendritic Molecular Aggregate. Molecular Crystals and Liquid Crystals, 2001, 371, 345-348.	0.3	2
236	Theoretical Study on the Polarizabilities of Two-Dimensionally-Grown Dendritic Molecular Aggregates: The Artichitecture- and Size-Dependency. Molecular Crystals and Liquid Crystals, 2001, 371, 215-218.	0.3	0
237	Third-order nonlinear optical properties of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. Journal of Chemical Physics, 2001, 115, 6780-6784.	1.2	10
238	Size-dependency of polarizabilities of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. Journal of Chemical Physics, 2001, 115, 1052-1059.	1.2	18
239	Theoretical studies on magnetic behavior in clusters by the genetic algorithms. International Journal of Quantum Chemistry, 2000, 80, 646-656.	1.0	4
240	Generalized spin density functional theory for noncollinear molecular magnetism. International Journal of Quantum Chemistry, 2000, 80, 664-671.	1.0	44
241	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.	1.0	28
242	MP2, Tamm-Dancoff, and RPA methods based on the generalized HF solution. International Journal of Quantum Chemistry, 2000, 80, 701-707.	1.0	17
243	Theoretical studies on superconducting and other phases: Triplet superconductivity, ferromagnetism, and ferromagnetic metal. International Journal of Quantum Chemistry, 2000, 80, 721-732.	1.0	15
244	Theoretical study on dependency of conductivity on structure of the proton- and electron-coupled system. International Journal of Quantum Chemistry, 2000, 80, 882-891.	1.0	6
245	A novel inclusion complex between molybdenum(II) fumarate and poly(ethylene glycol): first supramolecule formation between a microporous complex and an organic polymer. Polymers for Advanced Technologies, 2000, 11, 840-844.	1.6	12
246	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.	1.2	675
247	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.	9.5	133
248	Theoretical Study of the Antiferromagnetic Model Clusters for K₂MX₄ Type Solids. Molecular Crystals and Liquid Crystals, 2000, 343, 133-138.	0.3	16
249	Polarizabilities of Dendritic Molecular Aggregates: Contribution of Exciton Generation. Molecular Crystals and Liquid Crystals, 2000, 342, 303-308.	0.3	0
250	Theoretical Study on Magnetic Interactions of Mn-Ï€ Conjugated System. Molecular Crystals and Liquid Crystals, 2000, 342, 291-296.	0.3	0
251	Theoretical Studies on Quantum Tunneling of Spins in Cluster of Clusters. Molecular Crystals and Liquid Crystals, 2000, 342, 279-284.	0.3	0
252	Exciton Condensate in Model Dendrimers. Molecular Crystals and Liquid Crystals, 2000, 342, 273-278.	0.3	2

#	Article	IF	Citations
253	Local magnetic structure due to inhomogeneity of interaction inS=12antiferromagnetic chains. Physical Review B, 2000, 61, 4033-4040.	1.1	23
254	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.	1.2	105
255	Theoretical Study on Necessary Conditions for Reversible Photoinduced Magnetization: Cobalt-Iron Cyanide System. Molecular Crystals and Liquid Crystals, 2000, 343, 151-156.	0.3	6
256	Theoretical Studies on Magnetic Interaction of Di-Î¼-oxo Bridged Manganese Dimers. Molecular Crystals and Liquid Crystals, 2000, 343, 157-162.	0.3	5
257	Theoretical studies on anomalous phases of photodoped systems in two-band model. Journal of Chemical Physics, 2000, 113, 11237-11244.	1.2	31
258	Exciton Migration Pathways in Dendritic Molecular Aggregates. Molecular Crystals and Liquid Crystals, 2000, 342, 297-302.	0.3	0
259	Quantum-phase and information-entropy dynamics of a two-state molecular system interacting with strongly amplitude- and phase-squeezed fields. Journal of Chemical Physics, 2000, 112, 2769-2780.	1.2	14
260	Density-functional study of intramolecular ferromagnetic interaction throughm-phenylene coupling unit (II): Examination of functional dependence. Journal of Chemical Physics, 2000, 113, 10486-10504.	1.2	57
261	Local magnetic structures induced by inhomogeneities of the lattice inS=12bond-alternating chains and their response to a time-dependent magnetic field with noise. Physical Review B, 2000, 62, 9463-9471.	1.1	15
262	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
263	Synthesis and Gas-Occlusion Properties of Ruthenium(II,III) Dicarboxylates (Fumarate,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Liquid Crystals, 2000, 342, 199-204.	0.3	25
264	Theoretical Studies on Radical Spin Arrangements in the Cavity of Nanoporous Complexes. Molecular Crystals and Liquid Crystals, 2000, 343, 215-220.	0.3	6
265	Generalized Spin-Density Functional Calculation for the Spin Frustrated Systems. Molecular Crystals and Liquid Crystals, 2000, 343, 139-144.	0.3	3
266	Ab Initio Molecular Orbital Study on Thermal and Photochemical Reactions of 3-Furyl, 3-Pyrryl, and 3-Thienyl Fulgies. Molecular Crystals and Liquid Crystals, 2000, 345, 81-88.	0.3	6
267	Molecular Simulations of Argon, Nitrogen, and Hydrogen Adsorption in Microporous Complexes. Molecular Crystals and Liquid Crystals, 2000, 342, 285-290.	0.3	3
268	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
269	Synthesis and Characterization of Novel Inclusion Complexes between Microporous Molybdenum(II) Dicarboxylates and Organic Polymers. Macromolecules, 2000, 33, 6222-6227.	2.2	22
270	Frequency-dependent second hyperpolarizabilities in the time-dependent restricted open-shell Hartreeâ€“Fock theory: Application to the Li, Na, K, and N atoms. Journal of Chemical Physics, 2000, 112, 7903-7918.	1.2	8

#	Article	IF	Citations
271	Generalized spin density functional theory for noncollinear molecular magnetism. , 2000, 80, 664.		3
272	Theoretical study on dependency of conductivity on structure of the proton- and electron-coupled system. , 2000, 80, 882.		1
273	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
274	Theoretical Studies of the Pressure Effects for Î²-Phase of p-NPNN. Molecular Crystals and Liquid Crystals, 1999, 335, 623-632.	0.3	3
275	Theoretical Studies of Magnetic Interactions in 3â€², 5â€²-Dihydroxyphenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1999, 335, 633-642.	0.3	1
276	Calculation of frequency-dependent second hyperpolarizabilities for electric field induced second harmonic generation in the second-order Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1999, 111, 842-848.	1.2	13
277	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.	1.2	48
278	Theoretical Studies of Intra- and Inter- Magnetic Interactions in TMAO(1,3,5,7 - Tetramethyl - 2, 6-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.3	2
279	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. Molecular Crystals and Liquid Crystals, 1999, 337, 393-396.	0.3	0
280	Local Magnetic Structure of Layered Compounds Cu2(OD)3X with Exchangeable Acid Anion X Studied by Solid State High Resolution Deuterium NMR. Molecular Crystals and Liquid Crystals, 1999, 335, 11-21.	0.3	12
281	Theoretical studies on the magnetic quantum tunneling rates in Mn clusters by the path integral method. Chemical Physics Letters, 1999, 302, 418-424.	1.2	12
282	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.	0.5	68
283	Quantum Phase Dynamics of Interaction between Photon Field and Magnetic System: Effects of Magnetic Quantum Tunnelling. Optical Review, 1999, 6, 227-231.	1.2	2
284	Theoretical Studies on the Second Hyperpolarizabilities of Trithiapentalene and Its Donor and Acceptor Disubstituted Species. Optical Review, 1999, 6, 232-236.	1.2	1
285	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. Optical Review, 1999, 6, 237-241.	1.2	0
286	Electron correlation and structure dependencies of the second hyperpolarizability of ethylene. International Journal of Quantum Chemistry, 1999, 71, 177-183.	1.0	6
287	Numerical coupled Liouville approach: Application to second hyperpolarizability of molecular aggregate. International Journal of Quantum Chemistry, 1999, 71, 295-306.	1.0	3
288	CAS-SCF and density functional calculations of second hyperpolarizabilities for a nitronyl nitroxide radical. International Journal of Quantum Chemistry, 1999, 71, 329-336.	1.0	10

#	Article	IF	Citations
289	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.	1.0	26
290	Self-consistent-field calculations of molecular magnetic properties using gauge-invariant atomic orbitals. International Journal of Quantum Chemistry, 1999, 75, 637-643.	1.0	6
291	Visualization of two-body electron densities and wave functions of magnetic molecules. International Journal of Quantum Chemistry, 1999, 75, 645-654.	1.0	8
292	Density functional theory without the Born-Oppenheimer approximation. II. Green function techniques. International Journal of Quantum Chemistry, 1999, 75, 875-883.	1.0	20
293	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.	1.2	60
294	Third-Order Nonlinear Optical Properties of Ï€-Conjugated Systems Involving Sulfur Atoms: A Proposal of Multi-Property Materials Combining Conductivity and Unique Third-Order Nonlinearity. Molecular Crystals and Liquid Crystals, 1999, 337, 369-372.	0.3	2
295	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.	1.2	21
296	Calculation of frequency-dependent first hyperpolarizabilities using the second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1999, 110, 11720-11733.	1.2	18
297	Ab Initio Crystal Orbital Study of Ferromagnetic Interactions of Spins in Polymer Comprising Phenylenevinylene. Molecular Crystals and Liquid Crystals, 1999, 335, 613-622.	0.3	3
298	Dynamics of Magnetization for a System (S=3) with Strong Uniaxial Magnetocrystalline Anisotropy. Molecular Crystals and Liquid Crystals, 1999, 335, 593-602.	0.3	3
299	Magic Angle Spinning ¹H-NMR Study of the Spin Density Distribution of Pyridyl Nitronyl Nitroxides in the Crystalline Phase. Molecular Crystals and Liquid Crystals, 1999, 334, 295-304.	0.3	3
300	Density functional theory without the Bornâ€“Oppenheimer approximation. II. Green function techniques. , 1999, 75, 875.		1
301	An ab initio molecular orbital study of a binuclear dioxygen complex as a model of the binuclear active site in cytochrome c oxidase. Chemical Physics Letters, 1998, 294, 459-467.	1.2	13
302	Numerical coupled Liouville approach: Quantum dynamics of linear molecular aggregates under intense electric fields. International Journal of Quantum Chemistry, 1998, 70, 77-87.	1.0	0
303	Hyperpolarizabilities of one-dimensional Hn systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. International Journal of Quantum Chemistry, 1998, 70, 269-282.	1.0	10
304	Possibility of charge-mediated superconductors in the intermediate region of metal-insulator transitions. International Journal of Quantum Chemistry, 1998, 70, 1075-1084.	1.0	19
305	Density functional theory without the Born-Oppenheimer approximation and its application. International Journal of Quantum Chemistry, 1998, 70, 659-669.	1.0	54
306	Third-Order Nonlinear Optical Properties of a Stable Radical Species with Nitronyl Nitroxide Group. Molecular Crystals and Liquid Crystals, 1998, 315, 117-122.	0.3	9

#	Article	IF	Citations
307	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.	6.6	352
308	Numerical Coupled Liouville Approach:Â Dependence of Polarizability on Field Intensity and the Size of Linear Molecular Aggregates. Journal of Physical Chemistry A, 1998, 102, 6807-6811.	1.1	1
309	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.	2.0	25
310	Hyperpolarizabilities of oneâ€dimensional Hn systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. International Journal of Quantum Chemistry, 1998, 70, 269-282.	1.0	1
311	Density functional theory without the Bornâ€“Oppenheimer approximation and its application. International Journal of Quantum Chemistry, 1998, 70, 659-669.	1.0	3
312	Many-electron hyperpolarizability density analysis: Application to the dissociation processof one-dimensionalH2s. Physical Review A, 1997, 55, 1503-1513.	1.0	76
313	Path integral method by means of generalized coherent states and its numerical approach to molecular systems. I. Ensemble average of total energy. Journal of Chemical Physics, 1997, 107, 6283-6289.	1.2	9
314	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
315	Casci and Casscf Studies of Dinuclear Transition Metal Systems with Quadruple Metal-Metal Bonds (M=Cr(Ii), Mo(Ii)). Molecular Crystals and Liquid Crystals, 1997, 306, 321-330.	0.3	0
316	Theoretical Studies of Magnetic Interactions in 2â€², 5â€²-Dihydroxyphenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1997, 306, 151-160.	0.3	9
317	Theoretical Studies of Magnetic Interactions in P-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 Ï€-Conjugated Bis-Methylene Systems. Molecular Crystals and Liquid Crystals, 1997, 306, 475-486.	0.3	4
319	Magnetic Properties of Oxygen Physisorbed in Cu-Trans-1,4-Cyclohexanedicarboxylic Acid. Molecular Crystals and Liquid Crystals, 1997, 306, 1-7.	0.3	55
320	Magnetic Properties of Polymers Containing Paramagnetic Metalloporphyrins in Their Main Chain. Molecular Crystals and Liquid Crystals, 1997, 306, 25-32.	0.3	2
321	Solid State ¹H-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
322	Theoretical Study and Comparison with Experiments for Atacamite, Cu₂Cl(Oh)₃. Molecular Crystals and Liquid Crystals, 1997, 306, 33-40.	0.3	1
323	Magnetic Interaction Via Î²-Hydrogen Atoms in Tempo Derivatives. Molecular Crystals and Liquid Crystals, 1997, 306, 141-150.	0.3	16
324	Theoretical Studies on Hyperpolarizabelities of Nitroxide Species II. Second Hyperpolarizability of p-NPNN. Molecular Crystals and Liquid Crystals, 1997, 294, 251-254.	0.3	0

#	Article	IF	Citations
325	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.	1.1	132
326	Three Dimensional Wavepacket Simulation on the H Atom Scattering for the Full Reaction of CF₃H + Ar (³P) â†' CF₃* + H + Ar. Israel Journal of Chemistry, 1997, 37, 359-365.	1.0	0
327	Theoretical Studies of one Dimensional Tetranuclear Transition Metal Systems and their Clusters. Molecular Crystals and Liquid Crystals, 1997, 306, 463-474.	0.3	4
328	Theoretical study on rotational barriers of 1,3-dipoles and mechanisms of 1,3-dipolar reactions. , 1997, 2, 218-235.		6
329	Theoretical study on electronic structures of oxygenated dipoles and mechanisms of ozonolysis reactions. , 1997, 2, 236-252.		3
330	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.	1.0	23
331	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. International Journal of Quantum Chemistry, 1997, 65, 697-707.	1.0	3
332	CASSCF, MP2, and CASMP2 studies on addition reaction of singlet molecular oxygen to ethylene molecule. International Journal of Quantum Chemistry, 1997, 65, 787-801.	1.0	30
333	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.	1.0	47
334	Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order MÃ¸llerâ€“Plesset perturbation theory level based on the quasi-energy derivative method. , 1997, 65, 665.		1
335	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. , 1997, 65, 697.		1
336	Calculation of frequencyâ€dependent polarizabilities for openâ€shell systems at the secondâ€order MÃ¸llerâ€“Plesset perturbation theory level based on the quasiâ€energy derivative method. International Journal of Quantum Chemistry, 1997, 65, 665-677.	1.0	1
337	Theoretical Approaches to Molecular Magnetism. ACS Symposium Series, 1996, , 30-43.	0.5	12
338	Nonadiabatic treatment of molecular systems by the wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1261-1270.	1.0	4
339	Many-electron-wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1291-1301.	1.0	3
340	Theoretical Studies of Direct Exchange Couplings Between Transition Metal Ions I. Naked Binuclear Chromium(II) and Molybdenum (II) Systems. Molecular Crystals and Liquid Crystals, 1996, 286, 193-200.	0.3	5
341	Calculation of Magnetization by Path Integral Method II. Molecular Crystals and Liquid Crystals, 1996, 286, 177-184.	0.3	4
342	Calculation of Magnetization by Path Integral Method I. Molecular Crystals and Liquid Crystals, 1996, 286, 171-176.	0.3	4

#	Article	IF	Citations
343	Ab Initio mo Calculations of Superexchange Integrals For Transition-Metal Fluorides: MFM3+ (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
344	Theoretical Studies of Direct Exchange Couplings Between Transition Metal Ions II. Tetranuclear Transition Metal Systems. Molecular Crystals and Liquid Crystals, 1996, 286, 201-210.	0.3	6
345	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. Molecular Crystals and Liquid Crystals, 1996, 286, 43-50.	0.3	0
346	Theoretical Calculation of Effective Exchange Integrals for One-and Two-Dimensional Poly(Phenylenemethylene) Systems. Possibilities of Organic Ferro-and Ferri-Magnetic Solids. Molecular Crystals and Liquid Crystals, 1996, 279, 9-18.	0.3	9
347	Theoretical Studies on Nonlinear Optical Properties of Organometallic Conjugated Systems I: Static Third-Order Hyperpolarizabilities of First- Transition-Metal and Metal-Methylene Cations. Molecular Crystals and Liquid Crystals, 1996, 286, 159-164.	0.3	1
348	Theoretical Studies of the Ferromagnetic Inter-Molecular Interaction of P-Carboxylate Phenyl Nitronyl Nitroxide. Molecular Crystals and Liquid Crystals, 1996, 279, 29-38.	0.3	11
349	Magnetic Properties Of Basic Copper(?) Formates. Molecular Crystals and Liquid Crystals, 1996, 286, 17-22.	0.3	1
350	Molecular Design and Synthesis of Ferro-and Ferri-Magnetic Inorganic Polymers and Complexes with Tetrathiolate Ligands. Molecular Crystals and Liquid Crystals, 1996, 279, 1-8.	0.3	10
351	Theoretical Study of Effective Exchange Integrals for Ferromagnetic Phenylenevinylene Polymers with Nitroxdes. Possibilities of Organic Ferro-or Ferri-Magnetic Solids. Molecular Crystals and Liquid Crystals, 1996, 279, 19-28.	0.3	10
352	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.	1.2	30
353	CASSCF and CASPT2 calculations of hole-doped polycarbenes. Possibilities of organic ferromagnetic conductors and metals. Chemical Physics Letters, 1995, 233, 257-265.	1.2	52
354	New Cation-Diffusing Phase of (CH3NH3)5Bi2Cl11. Journal of the Physical Society of Japan, 1995, 64, 391-394.	0.7	7
355	Theoretical Studies of Spin Populations on Nitronyl Nitroxide, Phenyl Nitronyl Nitroxide and P-NPNN. Molecular Crystals and Liquid Crystals, 1995, 271, 19-28.	0.3	2
356	Spin Glass Behavior of Synthetic Atacamite, Cu₂Cl(OH)₃. Molecular Crystals and Liquid Crystals, 1995, 274, 113-118.	0.3	8
357	Ï€-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
358	Theoretical Approaches to Molecular Magnetism II: No-Overlap and Orientation Principles for Ferromagnetic Interactions. Molecular Crystals and Liquid Crystals, 1995, 272, 117-129.	0.3	8
359	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.	1.2	250
360	Magnetic Behavior of Polymers Containing Paramagnetic Metalloporphyrins. Molecular Crystals and Liquid Crystals, 1995, 273, 117-124.	0.3	6

#	Article	IF	Citations
361	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.	6.6	75
362	Theoretical Studies for Third-Order Hyperpolarizabilities of Alternant and Condensed-Ring Conjugated Systems I. Molecular Crystals and Liquid Crystals, 1994, 255, 139-148.	0.3	16
363	Theoretical studies on hyperpolarizabilities of nitroxide species I. , 1994, , .		0
364	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.	1.8	87
365	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. Chemical Physics Letters, 1994, 226, 372-380.	1.2	39
366	Effective exchange integrals for open-shell species by density functional methods. Chemical Physics Letters, 1994, 231, 25-33.	1.2	304
367	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
368	ESR and NMR study on the charge-transfer complexes of N-Ssalicylideneanilines containing NHO hydrogen bond as a dynamic function. , 1994, , .		0
369	High-spin ion radicals of polyenes and polyamines. A MO theoretical study. Chemical Physics Letters, 1993, 207, 9-14.	1.2	29
370	Instability in chemical bonds. II. Theoretical studies of exchange-coupled open-shell systems. International Journal of Quantum Chemistry, 1993, 48, 501-515.	1.0	35
371	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
372	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
373	New models for organic magnetic conductors or organic kondo and dense kondo systems. Synthetic Metals, 1991, 43, 3631-3634.	2.1	48
374	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.	1.0	51
375	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.	1.2	98
376	A general spin-orbital (GSO) description of antiferromagnetic spin couplings between four irons in iron-sulfur clusters. Chemical Physics Letters, 1990, 168, 56-62.	1.2	29
377	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.	1.2	32
378	Ab initiomolecular-orbital study on electron correlation effects inCuO6clusters relating to high-Tcsuperconductivity. Physical Review B, 1990, 42, 266-272.	1.1	18

#	Article	IF	Citations
379	CNDO/Sâ€'CI Calculations of Hyperpolarizabilities. III. Regular Polyenes, Charged Polyenes, Di-substituted Polyenes, Polydiacetylene and Related Species. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1990, 182, 1-15.	0.3	9
380	Ab Initio Calculations of Effective Exchange Integrals. Possibilities of Superparamagnetic, Mictomagnetic and Amorphous Feromagnetic States for Aggregates of Aromatic Free Radicals and Polymer Radicals. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1989, 176, 151-161.	0.3	12
381	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. Japanese Journal of Applied Physics, 1989, 28, L479-L482.	0.8	12
382	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.	1.2	63
383	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.	1.2	53
384	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.	1.2	720
385	Ab initio molecular orbital calculations of effective exchange integrals between transition metal ions. Chemical Physics Letters, 1988, 143, 371-376.	1.2	154
386	Extended Hartree-Fock (EHF) theory of chemical reactions. Theoretica Chimica Acta, 1988, 73, 337-364.	0.9	214
387	Ab initioMO Studies of the Hole Delocalization in Copper Oxides and Related Species: Necessity of the Extended Hubbard Model. Japanese Journal of Applied Physics, 1988, 27, L509-L512.	0.8	18
388	Possible Organic Analogues to Copper Oxides: Applications of a J-Model. Japanese Journal of Applied Physics, 1988, 27, L766-L769.	0.8	28
389	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.	0.8	40
390	A Universal MO-VB Approach to Electron and Spin Correlations in Copper-Oxide Clusters: NÃ©el Order, Spin Fluctuation and High-TcSuperconductivity. Japanese Journal of Applied Physics, 1988, 27, L393-L396.	0.8	10
391	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.	0.8	30
392	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.	2.1	109
393	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.	0.8	207
394	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.	2.1	36
395	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.	0.7	201
396	Ab-Initio Molecular Orbital Studies of Structure and Reactivity of Transition Metal-OXO Compounds. , 1986, , 155-184.		283

#	Article	IF	Citations
397	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
398	Orbital symmetry, orbital stability, and orbital pairing rules for organic reactions in the ground state. International Journal of Quantum Chemistry, 1982, 22, 459-484.	1.0	17
399	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. Chemical Physics Letters, 1981, 78, 566-571.	1.2	12
400	Theoretical studies of photo-oxidative cleavage reactions of nitrogen-activated C?C double bonds of enamines, indoles, and tryptamines. International Journal of Quantum Chemistry, 1981, 20, 393-406.	1.0	8
401	Ab initio UHF and UHF NO CI approaches for quasi-degenerate systems: methylene peroxide (CH2OO). Chemical Physics Letters, 1980, 71, 563-568.	1.2	57
402	Ab initio unrestricted Hartree-Fock (UHF) andUHF-natural orbitalCI studies of ozone. International Journal of Quantum Chemistry, 1980, 18, 101-106.	1.0	24
403	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.	1.2	50
404	Multireference (MR) configuration interaction (CI) approach for quasidegenerate systems. International Journal of Quantum Chemistry, 1980, 18, 269-284.	1.0	12
405	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.	1.2	54
406	Zwitterionic intermediates in enamine-singlet oxygen reactions. configuration-interaction studies on the indole-singlet oxygen reactions. Tetrahedron Letters, 1979, 20, 3433-3436.	0.7	12
407	Singlet unrestricted Hartree-Fock Slater (UHFS) model for unstable metalî—¸metal bonds. Chemical Physics Letters, 1979, 66, 395-399.	1.2	60
408	Distribution of odd electrons in ground-state molecules. Theoretica Chimica Acta, 1978, 48, 175-183.	0.9	292
409	Extended Hartree-Fock (EHF) theory in chemical reactions. Theoretica Chimica Acta, 1978, 48, 185-206.	0.9	61
410	Generalized molecular orbital (GMO) theories of organic reaction mechanisms. Orbital symmetry, orbital stability and orbital pairing rules. Chemical Physics, 1978, 29, 117-139.	0.9	41
411	Instability of the restricted Hartree-Fock (RHF) solution for the triplet state. Molecular Physics, 1978, 35, 33-49.	0.8	5
412	DODS natural orbital (NO) CI investigations of 1,3â€diradicals: CH2NHO, CH2OO, and CH2CH2O. Journal of Chemical Physics, 1978, 68, 4323-4325.	1.2	21
413	MOLECULAR ORBITALS OF ANTIAROMATIC MOLECULES: CYCLIC POLYMETHINES (CH)3and (CH)4. Chemistry Letters, 1977, 6, 971-974.	0.7	7
414	The spin-optimized SCF general spin orbitals. Theoretical formulation. Journal of Chemical Physics, 1977, 67, 2527.	1.2	9

#	Article	IF	Citations
415	Correlation effects in singlet biradical species. Chemical Physics, 1977, 19, 35-42.	0.9	32
416	Heisenberg models of radical reactions: Local spin (magnetic) symmetry conservations of biradical species. Chemical Physics, 1977, 20, 171-181.	0.9	34
417	Theoretical studies of free radical reactions IV. Selection rules. Chemical Physics, 1977, 25, 215-235.	0.9	23
418	Localized natural orbitals of unstable molecules: ozone. Chemical Physics Letters, 1977, 50, 266-270.	1.2	23
419	Interrelationships between the effective for the H3 radical. Chemical Physics Letters, 1977, 46, 360-365.	1.2	51
420	Generalized Hartree-Fock natural-orbital configuration-interaction (GHF NO CI) approach to unstable molecules: trimethylene. Chemical Physics Letters, 1977, 49, 555-559.	1.2	49
421	Heisenberg models of radical reactions. Theoretica Chimica Acta, 1977, 45, 1-20.	0.9	21
422	On the mechanisms of aromatic substitution reactions. Chemical Physics Letters, 1976, 44, 65-69.	1.2	26
423	Electron-transfer biradical intermediates in ground-state reactions. Chemical Physics Letters, 1976, 40, 347-352.	1.2	20
424	General spin structures of organic radicals. Chemical Physics Letters, 1975, 30, 288-292.	1.2	58
425	The electronic structures of biradicals in the unrestricted Hartree-Fock approximation. Chemical Physics Letters, 1975, 33, 330-335.	1.2	384
426	Electronic structures of antiaromatic molecules. Chemical Physics Letters, 1975, 35, 230-235.	1.2	88
427	Selection rule in free radical reactions. Chemical Physics Letters, 1974, 28, 93-97.	1.2	37
428	A molecular-orbital theoretical classification of reactions of singlet ground-state molecules. Chemical Physics Letters, 1973, 22, 461-465.	1.2	103
429	Mechanisms of the reactions of singlet molecular oxygen with olefins. Chemical Physics Letters, 1973, 22, 466-470.	1.2	51
430	Mechanistic characterization of the thermal ring-opening of three-membered cyclic compounds. Chemical Physics Letters, 1973, 22, 471-475.	1.2	44
431	Three-dimensional multi-layered optical memory using dye and Au(III) doped SiO/sub 2//TiO/sub 2/ sol-gel medium. , 0, , .		0
432	Nearsightedness-related indices of finite systems based on linear response function: one-dimensional cases. Molecular Physics, 0, , 1-9.	0.8	2

#	Article	IF	Citations
433	Approximate Spin Projection for Broken-Symmetry Method and Its Application. , 0, , .		10