Mitsuo Shoji

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1180368/publications.pdf

Version: 2024-02-01

144 papers	2,807 citations	201674 27 h-index	223800 46 g-index
144 all docs	144 docs citations	144 times ranked	1852 citing authors

#	Article	IF	Citations
1	A general algorithm for calculation of Heisenberg exchange integrals J in multispin systems. Chemical Physics Letters, 2006, 432, 343-347.	2.6	268
2	Theoretical illumination of water-inserted structures of the CaMn4O5 cluster in the S2 and S3 states of oxygen-evolving complex of photosystem II: full geometry optimizations by B3LYP hybrid density functional. Dalton Transactions, 2012, 41, 13727.	3.3	176
3	Approximately spin-projected geometry optimization method and its application to di-chromium systems. Chemical Physics Letters, 2007, 442, 445-450.	2.6	129
4	Chemical Equilibrium Models for the S₃ State of the Oxygen-Evolving Complex of Photosystem II. Inorganic Chemistry, 2016, 55, 502-511.	4.0	90
5	QM/MM study of the S2 to S3 transition reaction in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2015, 636, 172-179.	2.6	79
6	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn₄O₅ cluster of PSII refined to 1.9 Ã... Xâ€ray resolution. International Journal of Quantum Chemistry, 2012, 112, 253-276.	2.0	66
7	Full geometry optimizations of the mixedâ€valence CaMn₄O₄X(H₂O)₄ (X=OH or O) cluster in OEC of PS II: Degree of symmetry breaking of the labile Mnâ€Xâ€Mn bond revealed by several hybrid DFT calculations. International Journal of Quantum Chemistry, 2013, 113, 525-541.	2.0	60
8	The nature of chemical bonds of the CaMn₄O₅ cluster in oxygen evolving complex of photosystem II: Jahnâ€Teller distortion and its suppression by Ca doping in cubane structures. International Journal of Quantum Chemistry, 2013, 113, 453-473.	2.0	60
9	Electronic and spin structures of manganese clusters in the photosynthesis II system. Polyhedron, 2005, 24, 2767-2777.	2.2	58
10	Strong Coupling between the Hydrogen Bonding Environment and Redox Chemistry during the S₂ to S₃ Transition in the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2015, 119, 13922-13933.	2.6	51
11	Theory of chemical bonds in metalloenzymes I: Analytical and hybrid-DFT studies on oxo and hydroxo diiron cores. International Journal of Quantum Chemistry, 2004, 100, 887-906.	2.0	49
12	Theory of chemical bonds in metalloenzymes. XV. Local singlet and triplet diradical mechanisms for radical coupling reactions in the oxygen evolution complex. International Journal of Quantum Chemistry, 2010, 110, 3101-3128.	2.0	49
13	Theoretical insight in to hydrogen-bonding networks and proton wire for the CaMn4O5 cluster of photosystem II. Elongation of Mnâ€“Mn distances with hydrogen bonds. Catalysis Science and Technology, 2013, 3, 1831.	4.1	49
14	Theory of chemical bonds in metalloenzymes VI: Manganeseâ€“oxo bonds in the photosynthesis II system. Polyhedron, 2007, 26, 2216-2224.	2.2	48
15	Generalized approximate spin projection calculations of effective exchange integrals of the CaMn4O5 cluster in the S1 and S3 states of the oxygen evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11911-11923.	2.8	48
16	The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and ?-oxo-bridged manganese porphyrin dimer. International Journal of Quantum Chemistry, 2004, 100, 943-956.	2.0	42
17	Clinical Use of a Blood Substitute. New England Journal of Medicine, 1980, 303, 391-392.	27.0	40
18	Spin, Valence, and Structural Isomerism in the S₃ State of the Oxygen-Evolving Complex of Photosystem II as a Manifestation of Multimetallic Cooperativity. Journal of Chemical Theory and Computation, 2019, 15, 2375-2391.	5.3	40

#	Article	IF	Citations
19	A theoretical study of zero-field splitting of organic biradicals. Polyhedron, 2005, 24, 2708-2715.	2.2	37
20	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Feâ€“2S] cluster. International Journal of Quantum Chemistry, 2007, 107, 116-133.	2.0	33
21	Theory of chemical bonds in metalloenzymes XXI. Possible mechanisms of water oxidation in oxygen evolving complex of photosystem II. Molecular Physics, 2018, 116, 717-745.	1.7	33
22	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Feï£¿2S] clusters. International Journal of Quantum Chemistry, 2007, 107, 609-627.	2.0	32
23	Theoretical consideration of intensity of an xâ€ray microbeam formed by a hollow glass pipe. Review of Scientific Instruments, 1993, 64, 135-142.	1.3	31
24	Large-scale QM/MM calculations of the CaMn₄O₅ cluster in the S₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. Faraday Discussions, 2017, 198, 83-106.	3.2	31
25	Theoretical studies of the damage-free S1 structure of the CaMn4O5 cluster in oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2015, 623, 1-7.	2.6	29
26	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Feâ€“7S] core. International Journal of Quantum Chemistry, 2006, 106, 3288-3302.	2.0	28
27	Theoretical modelling of biomolecular systems I. Large-scale QM/MM calculations of hydrogen-bonding networks of the oxygen evolving complex of photosystem II. Molecular Physics, 2015, 113, 359-384.	1.7	28
28	Nonadiabatic one-electron transfer mechanism for the Oâ€“O bond formation in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2018, 698, 138-146.	2.6	28
29	Quantum spin correction scheme for ab initio spin-unrestricted solutions: Multiple bonds case. International Journal of Quantum Chemistry, 2005, 105, 605-614.	2.0	26
30	On the guiding principles for lucid understanding of the damage-free S1 structure of the CaMn4O5 cluster in the oxygen evolving complex of photosystem II. Chemical Physics Letters, 2015, 627, 44-52.	2.6	26
31	Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron-sulfur clusters. International Journal of Quantum Chemistry, 2005, 105, 628-644.	2.0	25
32	Geometric and electronic structures of the synthetic Mn₄CaO₄ model compound mimicking the photosynthetic oxygen-evolving complex. Physical Chemistry Chemical Physics, 2016, 18, 11330-11340.	2.8	25
33	Geometry optimization method based on approximate spin projection and its application to F₂, CH₂, CH₂OO, and active site of urease. International Journal of Quantum Chemistry, 2007, 107, 3094-3102.	2.0	24
34	Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Feâ€4S clusters. International Journal of Quantum Chemistry, 2008, 108, 2881-2887.	2.0	24
35	Large-Scale QM/MM Calculations of Hydrogen Bonding Networks for Proton Transfer and Water Inlet Channels for Water Oxidationâ€”Theoretical System Models of the Oxygen-Evolving Complex of Photosystem II. Advances in Quantum Chemistry, 2015, 70, 325-413.	0.8	23
36	The reaction mechanism of sarcosine oxidase elucidated using FMO and QM/MM methods. Physical Chemistry Chemical Physics, 2017, 19, 9811-9822.	2.8	22

#	Article	IF	Citations
37	A theoretical study of the formation of glycine via hydantoin intermediate in outer space environment. Chemical Physics Letters, 2017, 687, 178-183.	2.6	22
38	First-principles study of the formation of glycine-producing radicals from common interstellar species. Molecular Astrophysics, 2018, 10, 11-19.	1.6	22
39	Density functional study of manganese dimer. International Journal of Quantum Chemistry, 2007, 107, 3178-3190.	2.0	21
40	Theory of chemical bonds in metalloenzymes. XVII. Symmetry breaking in manganese cluster structures and chameleonic mechanisms for the Oï£¿O bond formation of water splitting reaction. International Journal of Quantum Chemistry, 2012, 112, 121-135.	2.0	21
41	Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in PhotosystemÂII. Journal of Physical Chemistry B, 2018, 122, 6491-6502.	2.6	21
42	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.	2.0	20
43	Hybrid-density functional study of magnetism and ligand control in Ni9 complexes. Chemical Physics Letters, 2006, 421, 483-487.	2.6	19
44	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.	1.7	18
45	A QM/MM Study of the <scp>l</scp>-Threonine Formation Reaction of Threonine Synthase: Implications into the Mechanism of the Reaction Specificity. Journal of the American Chemical Society, 2014, 136, 4525-4533.	13.7	18
46	An efficient initial guess formation of broken-symmetry solutions by using localized natural orbitals. Chemical Physics Letters, 2014, 608, 50-54.	2.6	17
47	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.	2.6	17
48	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.	2.0	16
49	Involvement of Propionate Side Chains of the Heme in Circular Dichroism of Myoglobin: Experimental and Theoretical Analyses. Journal of Physical Chemistry B, 2015, 119, 1275-1287.	2.6	16
50	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.	1.7	16
51	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.	3.3	16
52	Theoretical studies on magnetic interactions and charge-dope effects in one-dimensional Ni5 and Ni7 complexes. Polyhedron, 2005, 24, 2751-2757.	2.2	15
53	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.	2.0	15
54	Full geometry optimizations of the CaMn4O4 model cluster for the oxygen evolving complex of photosystem II. Chemical Physics Letters, 2015, 640, 23-30.	2.6	15

#	Article	IF	Citations
55	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.	2.6	15
56	Theoretical studies on ferrimagnetic behavior of TCNE and manganese porphyrin dimer. Polyhedron, 2005, 24, 2720-2725.	2.2	14
57	Theoretical study on the magnetic interactions of active site in hemerythrin. Polyhedron, 2005, 24, 2701-2707.	2.2	14
58	Extended Hartreeâ€“Fock theory of chemical reactions. VIII. Hydroxylation reactions by P450. International Journal of Quantum Chemistry, 2008, 108, 2991-3009.	2.0	14
59	Theoretical studies on the structure and effective exchange integral (Jab) of an active site in oxyhemocyanin (oxyHc) by using approximately spin-projected geometry optimization (AP-opt) method. Chemical Physics Letters, 2008, 456, 76-79.	2.6	14
60	Catalytic Mechanism of Nitrile Hydratase Subsequent to Cyclic Intermediate Formation: A QM/MM Study. Journal of Physical Chemistry B, 2016, 120, 3259-3266.	2.6	14
61	Redox Potentialâ€Dependent Formation of an Unusual Hisâ€“Trp Bond in Bilirubin Oxidase. Chemistry - A European Journal, 2018, 24, 18052-18058.	3.3	14
62	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.	5.2	14
63	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.	2.0	13
64	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.	2.6	13
65	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.	0.8	13
66	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.	2.0	12
67	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.	2.0	12
68	Exploring reaction pathways for the structural rearrangements of the Mn cluster induced by water binding in the S3 state of the oxygen evolving complex of photosystem II. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 405, 112905.	3.9	12
69	Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. International Journal of Quantum Chemistry, 2005, 105, 615-627.	2.0	11
70	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.	2.0	11
71	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.	2.5	11
72	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.	2.6	11

#	Article	IF	Citations
73	Neutron crystallography of copper amine oxidase reveals keto/enolate interconversion of the quinone cofactor and unusual proton sharing. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10818-10824.	7.1	11
74	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.	2.6	10
75	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.	1.9	10
76	Quantum dynamics of exciton recurrence motion in dendritic molecular aggregates. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 178, 264-270.	3.9	9
77	Assignments of the MÃ¶ssbauer spectra of an inorganic [8Feâ€“7S] complex based on the first-principle calculations. Chemical Physics Letters, 2007, 446, 228-232.	2.6	9
78	Theoretical studies on ferromagnetic behavior of [Cr(C5(CH3)5)2]+[TCNE]â¯ and [Mn(C5(CH3)5)2]+[TCNQ]â¯. Polyhedron, 2007, 26, 2135-2141.	2.2	9
79	Theoretical studies on relation among structures, electric structures and magnetic interactions in MMX complexes. Polyhedron, 2007, 26, 2154-2160.	2.2	9
80	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.	3.0	9
81	Ab initio studies on the zero-field splitting parameters of manganese porphyrin complexes. Polyhedron, 2007, 26, 2309-2312.	2.2	8
82	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.	2.2	8
83	Theory of chemical bonds in metalloenzymes - Manganese oxides clusters in the oxygen evolution center -. AIP Conference Proceedings, 2012, , .	0.4	8
84	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.	2.2	8
85	A QM/MM study of nitric oxide reductase-catalysed N₂O formation. Molecular Physics, 2014, 112, 393-397.	1.7	8
86	A QM/MM study of the initial steps of catalytic mechanism of nitrile hydratase. Chemical Physics Letters, 2015, 623, 8-13.	2.6	8
87	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
88	Photosubstitution Reaction of cis-[Ru(bpy)₂(CH₃CN)₂]²⁺ and cis-[Ru(bpy)₂(NH₃)₂]²⁺ in Aqueous Solution via Monoaqua Intermediate. Journal of Physical Chemistry A, 2019, 123, 2497-2502.	2.5	8
89	Theoretical study of the photodissociation reaction of methanol. Chemical Physics Letters, 2019, 714, 137-142.	2.6	8
90	Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase. RSC Advances, 2020, 10, 38631-38639.	3.6	8

#	Article	IF	Citations
91	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
92	Formulation of master equation approach involving spinâ€“phonon coupling: Toward an understanding of spin dynamics in magnetic dendrimers. Polyhedron, 2005, 24, 2653-2657.	2.2	7
93	Theoretical Investigation of the Magnetic Interactions of Ni9 Complexes. Journal of Physical Chemistry A, 2008, 112, 4020-4028.	2.5	7
94	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
95	Light absorption efficiencies of photosynthetic pigments: the dependence on spectral types of central stars. International Journal of Astrobiology, 2015, 14, 505-510.	1.6	7
96	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.	1.7	7
97	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.	1.7	7
98	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.	3.9	7
99	Weak O2 binding and strong H2O2 binding at the non-heme diiron center of trypanosome alternative oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148356.	1.0	7
100	Evaporation residue formation competing with the fission process in the197Au+16O,12C reactions and fission barriers at a specifiedJ window. Zeitschrift FÃ¼r Physik A, Atomic Nuclei, 1988, 331, 53-62.	0.3	6
101	Theoretical studies on magnetic interactions between Ni(II) ions in urease. Polyhedron, 2005, 24, 2778-2783.	2.2	6
102	Quantum spin correction scheme based on spin-correlation functional for Kohnâ€“Sham spin density functional theory. Journal of Magnetism and Magnetic Materials, 2007, 310, e492-e494.	2.3	6
103	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.	2.0	6
104	Molecular mechanisms of substrate specificities of uridine-cytidine kinase. Biophysics and Physicobiology, 2016, 13, 77-84.	1.0	6
105	Search for the ground states of Ising spin clusters by using the genetic algorithms. International Journal of Quantum Chemistry, 2005, 105, 645-654.	2.0	5
106	Quantum dynamic simulations for single molecular magnets using anisotropic spin models. Polyhedron, 2009, 28, 2092-2096.	2.2	5
107	Quantal cumulant dynamics for realâ€time simulations of quantum manyâ€body systems. International Journal of Quantum Chemistry, 2015, 115, 300-308.	2.0	5
108	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

#	Article	IF	Citations
109	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
110	The electronic structure and magnetic property of Î¼-hydroxo bridged manganese porphyrin dimer. European Physical Journal D, 2006, 38, 193-197.	1.3	4
111	A Theoretical Study on Redox Potential and pKa of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	3.2	4
112	A Practical Approach for Searching Stable Molecular Structures by Introducing Repulsive Interactions among Walkers. Bulletin of the Chemical Society of Japan, 2018, 91, 1465-1473.	3.2	4
113	Reaction mechanism of N-cyclopropylglycine oxidation by monomeric sarcosine oxidase. Physical Chemistry Chemical Physics, 2020, 22, 16552-16561.	2.8	4
114	Hybrid density-functional theory studies on stable polycarbenes. Polyhedron, 2003, 22, 2067-2076.	2.2	3
115	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.	2.0	3
116	Performance of the divide-and-conquer approach used as an initial guess. Chemical Physics Letters, 2015, 634, 181-187.	2.6	3
117	Molecular Mechanism of the Reaction Specificity in Threonine Synthase: Importance of the Substrate Conformations. Journal of Physical Chemistry B, 2017, 121, 5536-5543.	2.6	3
118	Structural Changes of the Trinuclear Copper Center in Bilirubin Oxidase upon Reduction. Molecules, 2019, 24, 76.	3.8	3
119	First-Principles Study of the Reaction Mechanism of CHO + H on Graphene Surface. Journal of Physical Chemistry A, 2019, 123, 5633-5639.	2.5	3
120	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.	1.7	3
121	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.	3.9	3
122	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.	3.9	3
123	Heme-bound tyrosine vibrations in hemoglobin M: Resonance Raman, crystallography, and DFT calculation. Biophysical Journal, 2022, 121, 2767-2780.	0.5	3
124	Ab initio GSO-DFT study of spin-frustrated transition metal systems. Polyhedron, 2005, 24, 2784-2788.	2.2	2
125	A GSOâ€“HDFT study of noncollinear spin structures of [2Feâ€“2S] cluster. Polyhedron, 2007, 26, 2335-2341.	2.2	2
126	Substrate-mediated proton relay mechanism for the religation reaction in topoisomerase II. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1759-1765.	3.5	2

#	Article	IF	Citations
127	Light absorption and excitation energy transfer calculations in primitive photosynthetic bacteria. Molecular Physics, 2015, 113, 1413-1421.	1.7	2
128	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. Molecular Physics, 2017, 115, 2154-2167.	1.7	2
129	UNO(ULO) active space for multireference calculations on classical and quantum computers. Revisit to the iron-sulfur complexes. Chemical Physics Letters, 2020, 746, 137252.	2.6	2
130	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.	1.7	2
131	Development of a New Molecular Visualization Package: Makiko. Journal of Computer Chemistry Japan, 2009, 8, 113-118.	0.1	2
132	Protonic Conduction in SrY0.5Ta0.5O3-Based Ceramics at Elevated Temperatures. , 1999, 3, 311-315.		1
133	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. Molecular Crystals and Liquid Crystals, 2006, 455, 135-141.	0.9	1
134	Theoretical studies on electronic structure and magnetic properties of mixedâ€valence uteroferrin active site. International Journal of Quantum Chemistry, 2011, 111, 702-710.	2.0	1
135	Calculation of the electron transfer coupling matrix element in diabatic reactions. International Journal of Quantum Chemistry, 2013, 113, 342-347.	2.0	1
136	Ab initio computations of zero-field splitting parameters and effective exchange integrals for single-molecule magnets (Mn12- and Mn11Cr-acetate clusters). Polyhedron, 2017, 136, 159-169.	2.2	1
137	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.	0.8	1
138	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.	2.2	0
139	A QM/MM study of the 5â€²-AMP DNA hydrolysis of aprataxin. Chemical Physics Letters, 2015, 631-632, 16-20.	2.6	0
140	Classical cumulant dynamics for statistical chemical physics. Molecular Simulation, 2017, 43, 1260-1268.	2.0	0
141	Reaction mechanism of non-enzymatic stereoselective formation of wine lactone. Chemical Physics Letters, 2019, 725, 114-118.	2.6	0
142	Reaction of threonine synthase with the substrate analogue 2-amino-5-phosphonopentanoate: implications into the proton transfer at the active site. Journal of Biochemistry, 2020, 167, 357-364.	1.7	0
143	Mechanism of Water Oxidation in Photosynthesis Elucidated by Interplay Between Experiment and Theory. Advances in Photosynthesis and Respiration, 2021, , 39-80.	1.0	0
144	The Reaction Mechanisms of O₂ Formation in Photosynthesis. Seibutsu Butsuri, 2018, 58, 127-133.	0.1	0