Toru Saito

List of Publications by Year in descending order

94 papers	1,641 citations	361413 20 h-index	345221 36 g-index
94 all docs	94 docs citations	94 times ranked	1367 citing authors

#	Article	IF	Citations
1	Approximately spin-projected geometry optimization method and its application to di-chromium systems. Chemical Physics Letters, 2007, 442, 445-450.	2.6	129
2	Possible mechanisms for the Oâ€“O bond formation in oxygen evolution reaction at the CaMn4O5(H2O)4 cluster of PSII refined to 1.9 Ã... X-ray resolution. Chemical Physics Letters, 2011, 511, 138-145.	2.6	96
3	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A1) by Broken-Symmetry Method. Journal of Physical Chemistry A, 2009, 113, 15041-15046.	2.5	68
4	Transition state optimization based on approximate spin-projection (AP) method. Chemical Physics Letters, 2009, 483, 168-171.	2.6	67
5	Labile electronic and spin states of the CaMn4O5 cluster in the PSII system refined to the 1.9 Ã... X-ray resolution. UB3LYP computational results. Chemical Physics Letters, 2011, 506, 98-103.	2.6	66
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	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
10	Structure and reactivity of the mixedâ€valence CaMn₄O₅(H₂O)₄ and CaMn₄O₄(OH)(H₂O)₄ clusters at oxygen evolution complex of photosystem II. Hybrid DFT (UB3LYP and UBHandHLYP) calculations. International Journal of Quantum Chemistry, 2012, 112, 321-343.	2.0	48
11	Reinvestigation of the Reaction of Ethylene and Singlet Oxygen by the Approximate Spin Projection Method. Comparison with Multireference Coupled-Cluster Calculations. Journal of Physical Chemistry A, 2010, 114, 7967-7974.	2.5	44
12	Analytical Gradients for Density Functional Calculations with Approximate Spin Projection. Journal of Physical Chemistry A, 2012, 116, 10864-10869.	2.5	44
13	Symmetry and broken symmetry in molecular orbital description of unstable molecules IV: comparison between single- and multi-reference computational results for antiaromtic molecules. Theoretical Chemistry Accounts, 2011, 130, 749-763.	1.4	40
14	Modification of MOF catalysts by manipulation of counter-ions: experimental and theoretical studies of photochemical hydrogen production from water over microporous diruthenium (II, III) coordination polymers. Supramolecular Chemistry, 2011, 23, 287-296.	1.2	32
15	Singletâ€“triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. Theoretical Chemistry Accounts, 2011, 130, 739-748.	1.4	30
16	Which hybrid GGA DFT is suitable for Cu2O2 systems if the spin contamination error is removed?. Chemical Physics, 2010, 368, 1-6.	1.9	25
17	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
18	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

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19	Multireference Character of 1,3-Dipolar Cycloaddition of Ozone with Ethylene and Acrylonitrile. Journal of Physical Chemistry A, 2010, 114, 12116-12123.	2.5	24
20	Heterogeneous catalase-like activity of gold(<scp>i</scp>)â€“cobalt(<scp>iii</scp>) metallosupramolecular ionic crystals. Chemical Science, 2017, 8, 2671-2676.	7.4	22
21	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
22	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
23	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.	2.6	20
24	A broken-symmetry study on the automerization of cyclobutadiene. Comparison with UNO- and DNO-MRCC methods. Chemical Physics Letters, 2010, 498, 253-258.	2.6	19
25	Theoretical investigation of the interaction between oxygen molecules and small Au clusters using approximately spin-projected geometry optimization (AP-opt) method. Catalysis Today, 2009, 143, 282-285.	4.4	18
26	Ab initio study of magnetic interactions of manganese-oxide clusters. Polyhedron, 2011, 30, 3256-3261.	2.2	18
27	Quantum Mechanics/Molecular Mechanics Study of Oxygen Binding in Hemocyanin. Journal of Physical Chemistry B, 2014, 118, 5034-5043.	2.6	18
28	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.	2.5	17
29	Computational Study of Catalytic Reaction of Quercetin 2,4-Dioxygenase. Journal of Physical Chemistry B, 2015, 119, 6952-6962.	2.6	16
30	Reparameterization of PM6 Applied to Organic Diradical Molecules. Journal of Physical Chemistry A, 2016, 120, 8750-8760.	2.5	16
31	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
32	UNOâ€•and ULOâ€MRCC(Mk), APâ€ŁCC and APâ€ŁBD approaches to diradical systems. International Journal of Quantum Chemistry, 2010, 110, 3015-3026.	2.0	15
33	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
34	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.	3.2	15
35	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
36	Performance of the coupled cluster and DFT methods for through-space magnetic interactions of nitroxide dimer. Chemical Physics Letters, 2012, 542, 19-25.	2.6	14

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37	Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals. Molecular Physics, 2017, 115, 2267-2284.	1.7	14
38	A Bis(Î¼â€oxido)dinickel(III) Complex with a Triplet Ground State. Angewandte Chemie - International Edition, 2018, 57, 7640-7643.	13.8	14
39	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
40	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
41	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. Polyhedron, 2009, 28, 1945-1949.	2.2	12
42	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
43	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
44	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.	3.2	11
45	MkMRCC, APUCC and APUBD approaches to 1,n-didehydropolyene diradicals: the nature of through-bond exchange interactions. Molecular Physics, 2010, 108, 2559-2578.	1.7	11
46	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.	2.0	10
47	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. Molecular Physics, 2010, 108, 2533-2541.	1.7	10
48	Theoretical Investigation for Heterojunction Effects in Polymer-stabilized Au Nanocluster Catalysis: Difference in Catalytic Activity between Au:PVP and Au:PAA. Chemistry Letters, 2016, 45, 344-346.	1.3	10
49	Approximate Spin Projection for Broken-Symmetry Method and Its Application. , 0, , .		10
50	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
51	Instability in Chemical Bonds from Broken-Symmetry Single-Reference to Symmetry-Adapted Multireference Approaches to Strongly Correlated Electron Systems. , 2009, , .		9
52	BS DFT and BS HDFT studies of Crï£¿Cr sextuple bond from the viewpoint of electron correlation effects. International Journal of Quantum Chemistry, 2009, 109, 3315-3324.	2.0	9
53	Theoretical studies on magnetic interactions between Cu(II) ions in hydroxypyridone nucleobases. Polyhedron, 2009, 28, 1714-1717.	2.2	9
54	Theoretical study on singlet oxygen adsorption onto surface of graphene-like aromatic hydrocarbon molecules. Polyhedron, 2011, 30, 3249-3255.	2.2	9

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55	Does B3LYP correctly describe magnetism of manganese complexes with various oxidation numbers and various structural motifs?. Chemical Physics Letters, 2012, 519-520, 134-140.	2.6	9
56	QM/MM Molecular Dynamics Simulations Revealed Catalytic Mechanism of Urease. Journal of Physical Chemistry B, 2022, 126, 2087-2097.	2.6	9
57	Electron Conductivity in Modified Models of Artificial Metalâ€“DNA Using Greenâ€™s Function-Based Elastic Scattering Theory. Bulletin of the Chemical Society of Japan, 2011, 84, 366-375.	3.2	8
58	Theoretical study of intra- and inter-chain magnetic interactions in [Ni(chxn)2Br]Br2. Polyhedron, 2011, 30, 3116-3120.	2.2	8
59	Theory of chemical bonds in metalloenzymes - Manganese oxides clusters in the oxygen evolution center -. AIP Conference Proceedings, 2012, , .	0.4	8
60	Theoretical Study of Electronic Properties of Phenalenyl Radical and Zethrene Diradical Species: Possibility of Triplet Oxygen Adsorption onto Graphene Surface. Bulletin of the Chemical Society of Japan, 2015, 88, 149-161.	3.2	8
61	Theoretical study of absorption spectrum of dirhodium tetracarboxylate complex [Rh2(CH3COO)4(H2O)2] in aqueous solution revisited. Supramolecular Chemistry, 2011, 23, 329-336.	1.2	7
62	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
63	Theoretical Investigation on the Au-Anchor Site in Phosphate-Doped Au/Al₂O₃Catalysts. E-Journal of Surface Science and Nanotechnology, 2015, 13, 380-384.	0.4	6
64	Assessment of semi-empirical molecular orbital calculations for describing magnetic interactions. Polyhedron, 2017, 136, 52-57.	2.2	6
65	Estimation of effective exchange integral value of polyradical systems based on the band calculation. International Journal of Quantum Chemistry, 2009, 109, 3632-3640.	2.0	5
66	Sequenceâ€dependent protonâ€transfer reaction in stacked GC pair III: The influence of proton transfer to conductivity. International Journal of Quantum Chemistry, 2010, 110, 2221-2230.	2.0	5
67	Combination of approximate spinâ€projection and spinâ€restricted calculations based on ONIOM method for geometry optimization of large biradical systems. International Journal of Quantum Chemistry, 2013, 113, 290-295.	2.0	5
68	Spinâ€projected QM/MM Free Energy Simulations for Oxidation Reaction of Guanine in Bâ€'DNA by Singlet Oxygen. ChemPhysChem, 2021, 22, 561-568.	2.1	5
69	Theoretical studies on electronic structures and magnetic interactions of K4[Pt2(pop)4X] Â· 2H2O (X =) Tj ETQq1 1 0.784314 rgBT /O	2.2	4
70	Development of approximately spin projected energy derivatives for biradical systems. International Journal of Quantum Chemistry, 2010, 110, 3053-3060.	2.0	4
71	QM/MM study of hydrolysis of arginine catalysed by arginase. Molecular Physics, 0, , 1-9.	1.7	4
72	A Bis(Î¼â€oxido)dinickel(III) Complex with a Triplet Ground State. Angewandte Chemie, 2018, 130, 7766-7769.	2.0	4

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73	Transition State Search Using rPM6: Iron- and Manganese-Catalyzed Oxidation Reactions as a Test Case. Bulletin of the Chemical Society of Japan, 2018, 91, 1377-1389.	3.2	4
74	Quantitative assessment of reparameterized PM6 (rPM6) for hydrogen abstraction reactions. Molecular Physics, 2020, 118, e1700313.	1.7	4
75	Singlet O2 Reactions with Radical Cations of 8-Bromoguanine and 8-Bromoguanosine: Guided-Ion Beam Mass Spectrometric Measurements and Theoretical Treatments. Journal of Physical Chemistry A, 2022, 126, 68-79.	2.5	4
76	Geometry Optimization without Spin Contamination Error - Approximately Spin Projected Optimization Method -. AIP Conference Proceedings, 2007, , .	0.4	3
77	Theoretical study of magnetic interaction between C60 anion radicals. Polyhedron, 2009, 28, 1750-1753.	2.2	3
78	Theoretical studies of the effect of orientation of ligands and spin contamination error on the chemical bonding in the FeO2 core in oxymyoglobin. Computational and Theoretical Chemistry, 2010, 954, 98-104.	1.5	3
79	Theoretical studies on the structural and magnetic property of arginase active site. Supramolecular Chemistry, 2011, 23, 22-28.	1.2	3
80	rPM6 Parameters for Manganese and Application to Transition State Search for Oxidation Reactions of Cyclohexene by Manganese(IV)-Oxo Species. Chemistry Letters, 2017, 46, 1567-1569.	1.3	3
81	Singlet-Triplet Energy Gaps in Binuclear Copper Complexes and Organic Diradicals by Approximate Spin Projected Spin-unrestricted Coupled Cluster Method. Chemistry Letters, 2019, 48, 1441-1444.	1.3	3
82	Singlet O₂ Oxidation of the Radical Cation versus the Dehydrogenated Neutral Radical of 9-Methylguanine in a Watsonâ€“Crick Base Pair. Consequences of Structural Context. Journal of Physical Chemistry B, 2022, 126, 5458-5472.	2.6	3
83	Theoretical studies on the electronic structure of the synthetic complex of soluble methanemonooxygenase intermediate Q. Supramolecular Chemistry, 2011, 23, 83-87.	1.2	2
84	Nearsightedness-related indices of finite systems based on linear response function: one-dimensional cases. Molecular Physics, 0, , 1-9.	1.7	2
85	Quantum mechanics study on synthetic model of copper-containing quercetin 2,4-dioxygenase. Polyhedron, 2017, 136, 45-51.	2.2	2
86	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. Molecular Physics, 2017, 115, 2154-2167.	1.7	2
87	Theoretical study of magnetic interaction in pyrazole-bridged dinuclear Cu(II) complex. Polyhedron, 2017, 136, 132-135.	2.2	2
88	rPM6 parameters for phosphorous and sulphur-containing open-shell molecules. Molecular Physics, 2018, 116, 602-610.	1.7	2
89	Density functional study of the magneto-structural correlations of manganese complexes, [Mn2O2H(salpn)2]+(2â^') (n= 0â€“2) from the viewpoint of the protonation modes of the bridging oxygen anions. Polyhedron, 2017, 136, 102-109.	2.2	1
90	Quantitative Assessment of rPM6 for Fluorine- and Chlorine-Containing Metal Complexes: Comparison with Experimental, First-Principles, and Other Semiempirical Results. Molecules, 2018, 23, 3332.	3.8	1

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91	3P-111 Theoretical studies on the electronic structure of the active site of Tyrosinase(The 46th Annual) Tj ETQq1 1 0.784314 rgBT /Over	0.1	0
92	Vibrational frequency without spin contamination error - Approximately spin projected force constant -. , 2012, , .		0
93	First principle calculations of effective exchange integrals: Comparison between SR (BS) and MR computational results. , 2015, , .		0
94	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.	0.2	0