Ryoichi Fukuda

List of Publications by Year
in descending order

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78 papers	1,992 citations	236925 25 h-index	276875 41 g-index
79 all docs	79 docs citations	79 times ranked	2017 citing authors

#	Article	IF	Citations
1	Dâ€“Dâ^'Ï€â€“A-Type Organic Dyes for Dye-Sensitized Solar Cells with a Potential for Direct Electron Injection and a High Extinction Coefficient: Synthesis, Characterization, and Theoretical Investigation. Journal of Physical Chemistry C, 2012, 116, 25653-25663.	3.1	153
2	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178.	18.8	118
3	Quasirelativistic theory for the magnetic shielding constant. I. Formulation of Douglasâ€“Krollâ€“Hess transformation for the magnetic field and its application to atomic systems. Journal of Chemical Physics, 2003, 118, 1015-1026.	3.0	108
4	Quasirelativistic theory for magnetic shielding constants. II. Gauge-including atomic orbitals and applications to molecules. Journal of Chemical Physics, 2003, 118, 1027-1035.	3.0	103
5	Formulation and implementation of direct algorithm for the symmetry-adapted cluster and symmetry-adapted clusterâ€“configuration interaction method. Journal of Chemical Physics, 2008, 128, 094105.	3.0	84
6	A Theoretical Investigation on CO Oxidation by Singleâ€Atom Catalysts M₁/Î³â€Al₂O₃ (M=Pd, Fe, Co, and Ni). ChemCatChem, 2017, 9, 1222-1229.	3.7	76
7	Symmetry-adapted cluster and symmetry-adapted cluster-configuration interaction method in the polarizable continuum model: Theory of the solvent effect on the electronic excitation of molecules in solution. Journal of Chemical Physics, 2010, 133, 024104.	3.0	71
8	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. Journal of Chemical Theory and Computation, 2013, 9, 2368-2379.	5.3	57
9	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted clusterâ€“configuration interaction method in the polarizable continuum model. Journal of Chemical Physics, 2011, 134, 104109.	3.0	51
10	Electronic transitions in liquid amides studied by using attenuated total reflection far-ultraviolet spectroscopy and quantum chemical calculations. Journal of Chemical Physics, 2013, 139, 154301.	3.0	41
11	Aerobic oxidation of methanol to formic acid on Au20â^': a theoretical study on the reaction mechanism. Physical Chemistry Chemical Physics, 2012, 14, 3103.	2.8	40
12	Diracâ€“Fock calculations of the magnetic shielding constants of protons and heavy nuclei in XH2 (X=O, S, Se, and Te): a comparison with quasi-relativistic calculations. Chemical Physics Letters, 2000, 321, 452-458.	2.6	39
13	Photoisomerization and Proton-Coupled Electron Transfer (PCET) Promoted Water Oxidation by Mononuclear Cyclometalated Ruthenium Catalysts. Inorganic Chemistry, 2012, 51, 5386-5392.	4.0	38
14	Excited states and electronic spectra of extended tetraazaporphyrins. Journal of Chemical Physics, 2010, 133, 144316.	3.0	37
15	Rydberg and Ï€â€“Ï€* Transitions in Film Surfaces of Various Kinds of Nylons Studied by Attenuated Total Reflection Far-Ultraviolet Spectroscopy and Quantum Chemical Calculations: Peak Shifts in the Spectra and Their Relation to Nylon Structure and Hydrogen Bondings. Journal of Physical Chemistry B, 2014, 118, 11855-11861.	2.6	37
16	Relativistic effects and the halogen dependencies in the13C chemical shifts of CH4?nIn, CH4?nBrn, CCl4?nIn, and CBr4?nIn (n=0-4). Journal of Computational Chemistry, 2001, 22, 528-536.	3.3	36
17	Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison Between TD-PBE0 and SAC-CI. Journal of Chemical Theory and Computation, 2014, 10, 3969-3979.	5.3	36
18	Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. ACS Omega, 2019, 4, 2596-2609.	3.5	36

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19	Symmetry-adapted-cluster/symmetry-adapted-cluster configuration interaction methodology extended to giant molecular systems: Ring molecular crystals. Journal of Chemical Physics, 2007, 126, 084104.	3.0	34
20	Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer Active Ï€-Conjugated Benzimidazole Compounds: Influence of Structural Rigidification by Ring Fusion. Journal of Organic Chemistry, 2017, 82, 12173-12180.	3.2	34
21	Cooperative H₂ Activation at Ag Cluster/Î¸-Al₂O₃(110) Dual Perimeter Sites: A Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 7996-8006.	3.1	31
22	Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SACâ€“CI) Method: Confined Electronic Excited States of Furan as a Test Case. Journal of Chemical Theory and Computation, 2015, 11, 2063-2076.	5.3	31
23	Relativistic configuration interaction and coupled cluster methods using four-component spinors: Magnetic shielding constants of HX and CH3X (X=F, Cl, Br, I). Chemical Physics Letters, 2005, 408, 150-156.	2.6	29
24	Quasirelativistic theory for the magnetic shielding constant. III. Quasirelativistic second-order MÃ¸llerâ€“Plesset perturbation theory and its application to tellurium compounds. Journal of Chemical Physics, 2005, 123, 044101.	3.0	28
25	Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. Journal of Computational Chemistry, 2013, 34, 2498-2501.	3.3	27
26	ESIPT emission behavior of methoxy-substituted 2-hydroxyphenylbenzimidazole isomers. New Journal of Chemistry, 2018, 42, 5923-5928.	2.8	27
27	Quasirelativistic study of125Te nuclear magnetic shielding constants and chemical shifts. Journal of Computational Chemistry, 2001, 22, 1502-1508.	3.3	25
28	Synthesis and Optical Properties of Imidazole- and Benzimidazole-Based Fused Ï€-Conjugated Compounds: Influence of Substituent, Counteranion, and Ï€-Conjugated System. Journal of Organic Chemistry, 2015, 80, 7172-7183.	3.2	25
29	How Can We Understand Au₈ Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au₂₄(ER)₂₀ and Au₂₀(ER)₁₆ (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602.	13.7	25
30	Reaction Behavior of the NO Molecule on the Surface of an M_n Particle (M = Ru,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Journal of Physical Chemistry A, 2019, 123, 7021-7033.	2.5	24
31	Symmetry and vibrationally resolved absorption spectra near the O K edge of N2O: Experiment and theory. Chemical Physics Letters, 2007, 435, 182-187.	2.6	23
32	Electronic excited states and electronic spectra of biphenyl: a study using many-body wavefunction methods and density functional theories. Physical Chemistry Chemical Physics, 2013, 15, 17426.	2.8	23
33	Efficiency of perturbation-selection and its orbital dependence in the SAC-CI calculations for valence excitations of medium-size molecules. Journal of Computational Chemistry, 2014, 35, 2163-2176.	3.3	20
34	Projected <scp>CAP</scp>/<scp>SAC</scp>â€<scp>CI</scp> method with smooth <scp>V</scp>oronoi potential for calculating resonance states. Journal of Computational Chemistry, 2016, 37, 242-249.	3.3	19
35	Mechanism of the aerobic oxidation of methanol to formic acid on Au₈^{â^’}: A DFT study. International Journal of Quantum Chemistry, 2013, 113, 428-436.	2.0	18
36	Dielsâ€“Alder Cycloaddition of Cyclopentadiene and C₆₀ at the Extreme High Pressure. Journal of Physical Chemistry A, 2017, 121, 4363-4371.	2.5	18

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37	Mechanisms for Solvatochromic Shifts of Free-Base Porphine Studied with Polarizable Continuum Models and Explicit Soluteâ€“Solvent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 470-480.	5.3	17
38	Quasi-Relativistic Study of 199Hg Nuclear Magnetic Shielding Constants of Dimethylmercury, Disilylmercury and Digermylmercury. Journal of Physical Chemistry A, 2001, 105, 128-133.	2.5	16
39	Optical absorption and fluorescence of PRODAN in solution: Quantum chemical study based on the symmetry-adapted cluster-configuration interaction method. Chemical Physics Letters, 2012, 552, 53-57.	2.6	16
40	Electronic Transitions in Conformationally Controlled Peralkylated Hexasilanes. ChemPhysChem, 2016, 17, 3010-3022.	2.1	16
41	Coreâ€“Shell versus Other Structures in Binary Cu_{38â€“n}M_n Nanoclusters (M = Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au; n = 1, 2, and 6): Theoretical Insight into Determining Factors. Journal of Physical Chemistry C, 2017, 121, 10514-10528.	3.1	16
42	Mechanism of NOâ€“CO reaction over highly dispersed cuprous oxide on Î³-alumina catalyst using a metalâ€“support interfacial site in the presence of oxygen: similarities to and differences from biological systems. Catalysis Science and Technology, 2018, 8, 3833-3845.	4.1	16
43	Electronic Transitions in Conformationally Controlled Tetrasilanes with a Wide Range of SiSiSiSi Dihedral Angles. Chemistry - A European Journal, 2014, 20, 9431-9441.	3.3	15
44	Comparing the performance of TDâ€ĐFT and SACâ€ĆI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. Journal of Computational Chemistry, 2017, 38, 1084-1092.	3.3	15
45	Structures of Bimetallic Copperâ€“Ruthenium Nanoparticles: Incoherent Interface and Surface Active Sites for Catalytic Nitric Oxide Dissociation. Journal of Physical Chemistry C, 2017, 121, 300-307.	3.1	15
46	Valence ionization spectra of group six metal hexacarbonyls studied by the symmetry-adapted cluster-configuration interaction method. Journal of Chemical Physics, 2009, 131, 174303.	3.0	14
47	Oxidation and Storage Mechanisms for Nitrogen Oxides on Variously Terminated (001) Surfaces of SrFeO_{3â^Î´} and Sr₃Fe₂O_{7â^Î´} Perovskites. ACS Applied Materials & Interfaces, 2021, 13, 7216-7226.	8.0	14
48	Electronic excitations of C60 fullerene calculated using the ab initio cluster expansion method. Journal of Chemical Physics, 2012, 137, 134304.	3.0	13
49	Comparative Study of C^{â§}N and N^{â§}C Type Cyclometalated Ruthenium Complexes with a NAD⁺/NADH Function. Inorganic Chemistry, 2012, 51, 8091-8102.	4.0	13
50	Theoretical Study on the Excited Electronic States of Coronene and Its Ï€-Extended Molecules Using the Symmetry-Adapted Cluster-Configuration Interaction Method. Bulletin of the Chemical Society of Japan, 2013, 86, 445-451.	3.2	13
51	Electronic spectra and photodissociation of vinyl chloride: A symmetry-adapted cluster configuration interaction study. Journal of Chemical Physics, 2006, 124, 034312.	3.0	11
52	Vibration-induced suppression of valence-Rydberg mixing in the O1sâ†'nsÏƒRydberg series inN2O. Physical Review A, 2008, 77, .	2.5	11
53	Valence ionized states of iron pentacarbonyl and Î·5-cyclopentadienyl cobaltâ€‰dicarbonylâ€‰studiedâ€‰byâ€‰symmetry-adaptedâ€‰cluster-configuration interaction calculation and collision-energy resolved Penning ionization electron spectroscopy. Journal of Chemical Physics, 2010, 132, 084302.	3.0	11
54	Spectroscopy of sodium atom in liquid helium cluster: a symmetry adapted cluster-configuration interaction (SAC-CI) study. Theoretical Chemistry Accounts, 2007, 118, 437-441.	1.4	10

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55	Excited-state geometries and vibrational frequencies studied using the analytical energy gradients of the direct symmetry-adapted clusterâ€“configuration interaction method. I. HAX-type molecules. Journal of Chemical Physics, 2011, 135, 044316.	3.0	10
56	Electronic excitation spectra of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model with perturbative approach. Journal of Chemical Physics, 2014, 140, 064114.	3.0	10
57	An efficient computational scheme for electronic excitation spectra of molecules in solution using the symmetry-adapted clusterâ€“configuration interaction method: The accuracy of excitation energies and intuitive charge-transfer indices. Journal of Chemical Physics, 2014, 141, 154104.	3.0	10
58	Excited states and electronic spectra of annulated dinuclear free-base phthalocyanines: A theoretical study on near-infrared-absorbing dyes. Journal of Chemical Physics, 2012, 136, 114304.	3.0	9
59	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. Journal of Computational Chemistry, 2019, 40, 181-190.	3.3	9
60	Protonâ€Induced Generation of Remote Nâ€Heterocyclic Carbeneâ€“Ru Complexes. Chemistry - A European Journal, 2015, 21, 106-110.	3.3	8
61	A catalyzed E/Z isomerization mechanism of stilbene using para-benzoquinone as a triplet sensitizer. Physical Chemistry Chemical Physics, 2022, 24, 1712-1721.	2.8	7
62	Synthesis and Optical Properties of Fused Ï€-Conjugated Imidazole Compounds. Chemistry Letters, 2017, 46, 1372-1375.	1.3	6
63	Quantum Chemical Study on the High-Pressure Effect for [4 + 4] Retrocycloaddition of Anthracene Cyclophane Photodimer. Journal of Physical Chemistry C, 2019, 123, 4493-4501.	3.1	6
64	Identification of hydrogen species on Pt/Al₂O₃ by in situ inelastic neutron scattering and their reactivity with ethylene. Catalysis Science and Technology, 2021, 11, 116-123.	4.1	6
65	Photophysical Properties and Photochemistry ofEE-,EZ-, andZZ-1,4-Dimethoxy-2,5-bis[2-(thien-2-yl)ethenyl] Benzene in Solution: Theory and Experiment. Journal of Physical Chemistry A, 2012, 116, 924-937.	2.5	5
66	Quantum Chemical Computation-Driven Development of Cu-Shellâ€“Ru-Core Nanoparticle Catalyst for NO Reduction Reaction. Journal of Physical Chemistry C, 2019, 123, 20251-20256.	3.1	5
67	Theoretical study of the electronic excitations of free-base porphyrinâ€“Ar2 van der Waals complexes. Journal of Chemical Physics, 2013, 139, 074303.	3.0	4
68	Electronic excitation and ionization behavior of N-hydroxypyridine-2(1H)-thione and its deprotonated anion in a polarizable medium studied using quantum chemical computations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
69	Photophysical properties of fluorescent imaging biological probes of nucleic acids: SACâ€CI and TDâ€DFT Study. Journal of Computational Chemistry, 2019, 40, 127-134.	3.3	4
70	Theoretical spectroscopy of O 1s and N 1s excited states of N₂O. Journal of Physics: Conference Series, 2011, 288, 012024.	0.4	3
71	Electronic excitation of molecules in solution calculated using the symmetry-adapted clusterâ€“configuration interaction method in the polarizable continuum model. AIP Conference Proceedings, 2015, , .	0.4	3
72	An analysis of valence electronic structure from a viewpoint of resonance theory: Tautomerization of formamide and diazadiboretidine. Journal of Computational Chemistry, 2021, 42, 1662-1669.	3.3	3

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73	Electronic excited states of macrocyclic compounds: direct SAC-CI study. Procedia Computer Science, 2011, 4, 1129-1134.	2.0	1
74	Symmetry and vibrationally resolved absorption spectra near theNâ€,Kedges ofN2O: Experiment and theory. Physical Review A, 2011, 83, .	2.5	1
75	Pseudo-Jahn-Teller effect on the lowest triplet state of para-benzoquinone involving inequivalent carbonyl bonds. Chemical Physics Letters, 2020, 741, 137072.	2.6	1
76	GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMILTONIANS. Recent Advances in Computational, 2004, , 191-220.	0.8	0
77	Electronic Structure and Stability of Binary Metal Cluster with Core-Shell Structure: Theoretical Approach. Journal of Computer Chemistry Japan, 2019, 18, 38-48.	0.1	0
78	Electronic Origin of Catalytic Nitric Oxide Reduction upon Small Rhodium and Copper Clusters. Journal of Computer Chemistry Japan, 2019, 18, 95-101.	0.1	0