Masahiko Hada

List of Publications by Year in Descending Order

190 papers	3,982 citations	36 h-index	50 g-index
201 ext. papers	4,314 ext. citations	3.9 avg, IF	5.37 L-index

#	Paper	IF	Citations
190	Rate-Limiting Step of Epoxidation Reaction of the Oxoiron(IV) Porphyrin Cation Radical Complex: Electron Transfer Coupled Bond Formation Mechanism. *Inorganic Chemistry*, **2021**, 60, 17687-17698	5.1	1
189	Density Functional Study of Metal-to-Ligand Charge Transfer and Hole-Hopping in Ruthenium(II) Complexes with Alkyl-Substituted Bipyridine Ligands. *ACS Omega*, **2021**, 6, 55-64	3.9	3
188	Theoretical Studies of Reaction Mechanisms for Half-Titanocene-Catalyzed Styrene Polymerization, Ethylene Polymerization, and Styrene Ethylene Copolymerization: Roles of the Neutral Ti(III) and the Cationic Ti(IV) Species. *Organometallics*, **2021**, 40, 643-653	3.8	
187	13C NMR chemical shifts in substituted benzenes: analysis using natural perturbation orbitals and substitution effects. *Molecular Physics*, **2021**, 119, e1843722	1.7	
186	Semi-Quantitative Calculations of Nucleus-Independent Chemical Shift (NICS) Using a One-Dimensional Ring Model. *Journal of Computer Chemistry Japan*, **2021**, 20, A2-A10	0.2	
185	-Substitution Activates Oxoiron(IV) Porphyrin Cation Radical Complex More Than Pyrrole- Substitution for Atom Transfer Reaction. *Inorganic Chemistry*, **2021**, 60, 3207-3217	5.1	7
184	Density Functional Study on Compounds to Accelerate the Electron Capture Decay of Be. *Journal of Physical Chemistry A*, **2021**, 125, 6356-6361	2.8	
183	Insights into the electronic structure and mechanism of norcarane hydroxylation by OxoMn(V) porphyrin complexes: A density functional theory study. *Journal of Computational Chemistry*, **2021**, 42, 1920-1928	3.5	0
182	Ab initio and steady-state models for uranium isotope fractionation in multi-step biotic and abiotic reduction. *Geochimica Et Cosmochimica Acta*, **2021**, 307, 212-227	5.5	2
181	Synthesis, characterization, and reactivity of oxoiron(IV) porphyrin cation radical complexes bearing cationic N-methyl-2-pyridinium group. *Journal of Inorganic Biochemistry*, **2021**, 223, 111542	4.2	0
180	DFT insight into axial ligand effects on electronic structure and mechanistic reactivity of oxoiron(iv) porphyrin. *Physical Chemistry Chemical Physics*, **2020**, 22, 12173-12179	3.6	4
179	Exploring the Relationship between Effective Mass, Transient Photoconductivity, and Photocatalytic Activity of SrxPb1 BiO2Cl (x = 0 1) Oxyhalides. *Chemistry of Materials*, **2020**, 32, 4166-4173	9.6	12
178	Experimental and Theoretical Investigation of the Role of Bismuth in Promoting the Selective Oxidation of Glycerol over Supported Pt Bi Catalyst under Mild Conditions. *ACS Catalysis*, **2020**, 10, 6071-6083	13.1	22
177	Surface-enhanced Raman scattering of M -pyrazine-M (M = Cu, Ag, Au): Analysis by natural perturbation orbitals and density functional theory functional dependence. *Journal of Computational Chemistry*, **2020**, 41, 1628-1637	3.5	2
176	Accurate determination of the enhancement factor X for the nuclear Schiff moment in 205TlF molecule based on the four-component relativistic coupled-cluster theory. *Molecular Physics*, **2020**, 118, e1767814	1.7	2
175	Relativistic coupled-cluster study of diatomic metal-alkali-metal molecules for electron electric dipole moment searches. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2020**, 53, 015102	1.3	2
174	Time-dependent DFT study of the K-edge spectra of vanadium and titanium complexes: effects of chloride ligands on pre-edge features. *Physical Chemistry Chemical Physics*, **2020**, 22, 674-682	3.6	9

173	Effect of External Electric Fields on the Oxidation Reaction of Olefins by Fe(IV)OCl Porphyrin Complexes. *Bulletin of the Chemical Society of Japan*, **2020**, 93, 187-193	5.1	8
172	Transition-Metal Capping to Suppress Back-Donation to Enhance Donor Ability. *Organometallics*, **2020**, 39, 4191-4194	3.8	5
171	Molecular structure and basic spectroscopic properties of 3-selenocyanatoindole: An important reference compound in organoselenium research. *Tetrahedron*, **2019**, 75, 130551	2.4	1
170	Factors influencing the photoelectrochemical device performance sensitized by ruthenium polypyridyl dyes. *Dalton Transactions*, **2019**, 48, 688-695	4.3	11
169	Experimental and theoretical studies of the porphyrin ligand effect on the electronic structure and reactivity of oxoiron(iv) porphyrin cation-radical complexes. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 483-494	3.7	15
168	The Role of Relativistic Many-Body Theory in Electron Electric Dipole Moment Searches Using Cold Molecules. *Atoms*, **2019**, 7, 58	2.1	
167	Merits of heavy-heavy diatomic molecules for electron electric-dipole-moment searches. *Physical Review A*, **2019**, 99,	2.6	8
166	Ultracold mercury alkali-metal molecules for electron-electric-dipole-moment searches. *Physical Review A*, **2019**, 99,	2.6	6
165	Substitution effects on olefin epoxidation catalyzed by Oxoiron(IV) porphyrin cation radical complexes: A dft study. *Journal of Computational Chemistry*, **2019**, 40, 1780-1788	3.5	7
164	Computational Study on the Search for Non-Fullerene Acceptors, Examination of Interface Geometry, and Investigation of Electron Transfer. *Journal of Physical Chemistry C*, **2019**, 123, 17678-17685	3.8	6
163	Inverted Sandwich Rh Complex Bearing a Plumbole Ligand and Its Catalytic Activity. *Organometallics*, **2019**, 38, 3099-3103	3.8	9
162	C and Pb NMR Chemical Shifts of Dirhodio- and Dilithioplumbole Complexes: A Quantum Chemical Assessment. *Inorganic Chemistry*, **2019**, 58, 14708-14719	5.1	
161	Alternative materials for perovskite solar cells from materials informatics. *Physical Review Materials* , **2019**, 3,	3.2	7
160	Functionalization of Endohedral Metallofullerenes toward Improving Barrier Height for the Relaxation of Magnetization for Dy@C-X (X = CF, CNPh). *Inorganic Chemistry*, **2019**, 58, 1208-1215	5.1	4
159	Can large active-space CASSCF calculation make sense to the reaction analysis of iron complex? A benchmark study of methane oxidation reaction by FeO. *Journal of Computational Chemistry*, **2019**, 40, 414-420	3.5	2
158	Extrapolation of polymer gap by combining cluster and periodic boundary condition calculations with Hckel theory. *Chemical Physics Letters*, **2018**, 707, 44-48	2.5	3
157	Anomalous Dielectric Behavior of a Pb/Sn Perovskite: Effect of Trapped Charges on Complex Photoconductivity. *ACS Photonics*, **2018**, 5, 3189-3197	6.3	17
156	First-Principles Calculations of the Rotational Motion and Hydrogen Bond Capability of Large Organic Cations in Hybrid Perovskites. *Journal of Physical Chemistry C*, **2018**, 122, 15966-15972	3.8	9

155	A theoretical study on the size-dependence of ground-state proton transfer in phenol-ammonia clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 3265-3276	3.6	5
154	Enhancement factors of parity- and time-reversal-violating effects for monofluorides. *Physical Review A*, **2018**, 98,	2.6	12
153	Synthesis and reactivity of a ruthenocene-type complex bearing an aromatic ligand with the heaviest group 14 element. *Chemical Science*, **2017**, 8, 3092-3097	9.4	16
152	Rotational Energy Barriers and Relaxation Times of the Organic Cation in Cubic Methylammonium Lead/Tin Halide Perovskites from First Principles. *Journal of Physical Chemistry C*, **2017**, 121, 14051-14059	3.8	19
151	Calculations of nuclear magnetic shielding constants based on the exact two-component relativistic method. *Journal of Chemical Physics*, **2017**, 147, 154104	3.9	14
150	Quantum Chemical Studies on Electron-Accepting Overcrowded Ethylene with a Polarizable Skeleton. *Journal of Physical Chemistry A*, **2017**, 121, 7797-7806	2.8	2
149	Theoretical Study of Formulation of Hyperfine Coupling Constant in Four-component Relativistic Framework. *Journal of Computer Chemistry Japan*, **2017**, 16, 81-82	0.2	
148	Analysis of large effective electric fields of weakly polar molecules for electron electric-dipole-moment searches. *Physical Review A*, **2017**, 95,	2.6	10
147	Theoretical Insights into the Electronic Structures and Stability of Dimetallofullerenes M2@Ih-C80. *Journal of Physical Chemistry C*, **2017**, 121, 18169-18177	3.8	12
146	Quantum Chemical Study on Endohedral Heteronuclear Dimetallofullerene M1M2@Ih-C80 toward Molecular Design. *Journal of Physical Chemistry C*, **2017**, 121, 27700-27708	3.8	3
145	Theoretical Study on Rotational Controllability of Organic Cations in Organic–Inorganic Hybrid Perovskites: Hydrogen Bonds and Halogen Substitution. *Journal of Physical Chemistry C*, **2017**, 121, 26188-26195	3.8	14
144	Vanadium NMR Chemical Shifts of (Imido)vanadium(V) Dichloride Complexes with Imidazolin-2-iminato and Imidazolidin-2-iminato Ligands: Cooperation with Quantum-Chemical Calculations and Multiple Linear Regression Analyses. *Journal of Physical Chemistry A*, **2017**, 121, 9099-9105	2.8	3
143	Anisotropic Crystals Based on a Main-Group Coordination Polymer with Alignment of Rigid Skeletons. *Organometallics*, **2017**, 36, 2487-2490	3.8	3
142	Automatic High-Throughput Screening Scheme for Organic Photovoltaics: Estimating the Orbital Energies of Polymers from Oligomers and Evaluating the Photovoltaic Characteristics. *Journal of Physical Chemistry C*, **2017**, 121, 28275-28286	3.8	17
141	Analysis of Electron Spin Density Induced by External Static Magnetic Field in Closed-shell Heavy Atomic Systems. *Journal of Computer Chemistry Japan*, **2017**, 16, 91-92	0.2	
140	Theoretical study of the infrared frequencies of crystalline methyl acetate under interstellar medium conditions. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 153, 415-21	4.4	1
139	The Origin of Relative Stability of Di-μ-oxo M M Chiral Salen Complexes [M M = Ti(IV) Ti(IV), V(IV) V(IV), Cr(IV) Cr(IV), and Mn(IV) Mn(IV)]: A Quantum-Chemical Analysis. *Bulletin of the Chemical Society of Japan*, **2016**, 89, 447-454	5.1	1
138	Correlating Magnetic Exchange in Dinuclear Bis(phenolate)-Bridged Complexes: A Computational Perspective. *Bulletin of the Chemical Society of Japan*, **2016**, 89, 657-665	5.1	8

137	Relativistic coupled-cluster calculation of the electron-nucleus scalar-pseudoscalar interaction constant Ws in YbF. *Physical Review A*, **2016**, 93,	2.6	25
136	Theoretical Design for Near-infrared Light Absorption of N3-skeleton Dye: Spin-forbidden Excitation. *Journal of Computer Chemistry Japan*, **2016**, 15, 77-78	0.2	
135	Design of spin-forbidden transitions for polypyridyl metal complexes by time-dependent density functional theory including spin-orbit interaction. *Physical Chemistry Chemical Physics*, **2016**, 18, 14466-78	3.6	2
134	The functional role of the structure of the dioxo-isobacteriochlorin in the catalytic site of cytochrome cd for the reduction of nitrite. *Chemical Science*, **2016**, 7, 2896-2906	9.4	16
133	Heavy Element Effects in the Diagonal Born-Oppenheimer Correction within a Relativistic Spin-Free Hamiltonian. *Journal of Physical Chemistry A*, **2016**, 120, 2150-9	2.8	5
132	Determination of genotoxic potential by comparison of structurally related azo dyes using DNA repair-deficient DT40 mutant panels. *Chemosphere*, **2016**, 164, 106-112	8.4	5
131	Comprehensive Understanding of Structure-Controlling Factors of a Zinc Tetraphenylporphyrin Thin Film Using pMAIRS and GIXD Techniques. *Chemistry - A European Journal*, **2016**, 22, 16539-16546	4.8	20
130	An ab initio study of nuclear volume effects for isotope fractionations using two-component relativistic methods. *Journal of Computational Chemistry*, **2015**, 36, 816-20	3.5	6
129	Infrared spectra and chemical abundance of methyl propionate in icy astrochemical conditions. *Monthly Notices of the Royal Astronomical Society*, **2015**, 448, 1372-1377	4.3	9
128	Gauge-origin dependence of NMR shielding constants in the Douglas□Kroll□Hess method. *Chemical Physics Letters*, **2015**, 618, 132-141	2.5	4
127	Di-□xo dimetal core of Mn(IV) and Ti(IV) as a linker between two chiral salen complexes leading to the stereoselective formation of different M- and P-helical structures. *Inorganic Chemistry*, **2014**, 53, 1070-9	5.1	14
126	Application of relativistic coupled-cluster theory to the effective electric field in YbF. *Physical Review A*, **2014**, 90,	2.6	45
125	Characterizing of variation in the proton-to-electron mass ratio via precise measurements of molecular vibrational transition frequencies. *Journal of Molecular Spectroscopy*, **2014**, 300, 99-107	1.3	13
124	Dipole polarizability of alkali-metal (Na, K, Rb)-alkaline-earth-metal (Ca, Sr) polar molecules: prospects for alignment. *Journal of Chemical Physics*, **2014**, 140, 224303	3.9	25
123	Test of mp/me changes using vibrational transitions in N2+. *Physical Review A*, **2014**, 89,	2.6	40
122	Quantum-chemical analyses of aromaticity, UV spectra, and NMR chemical shifts in plumbacyclopentadienylidenes stabilized by Lewis bases. *Journal of Computational Chemistry*, **2014**, 35, 847-53	3.5	7
121	Theoretical Study of Isotope Enrichment Caused by Nuclear Volume Effect. *Journal of Computer Chemistry Japan*, **2014**, 13, 92-104	0.2	3
120	Diagonal Born-Oppenheimer Correction Based on Spin-Free Relativistic Hamiltonians. *Journal of Computer Chemistry Japan*, **2014**, 13, 229-232	0.2	1

119	Oxygen-atom transfer from iodosylarene adducts of a manganese(IV) salen complex: effect of arenes and anions on I(III) of the coordinated iodosylarene. *Inorganic Chemistry*, **2013**, 52, 9557-66	5.1	34
118	The Douglas□Kroll□Hess method based on vector-potential-including Foldy□Wouthuysen transformation: Application to NMR shielding tensor. *Chemical Physics Letters*, **2013**, 580, 145-151	2.5	6
117	Ab initio study of ground and excited states of 6Li40Ca and 6Li88Sr molecules. *Journal of Chemical Physics*, **2013**, 138, 194307	3.9	16
116	Sensitivity of vibrational spectroscopy of optically trapped SrLi and CaLi molecules to variations inmp/me. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2013**, 46, 025001	1.3	28
115	Synthesis, structure, and reactivity of Lewis base stabilized plumbacyclopentadienylidenes. *Chemistry - A European Journal*, **2013**, 19, 16946-53	4.8	26
114	Ab initio study on potential energy curves of electronic ground and excited states of 40CaH+ molecule. *Chemical Physics Letters*, **2012**, 521, 31-35	2.5	16
113	Nuclear Magnetic Shielding and Aromaticity of [18]Annulene and Its Quasi-M□bius-Type Analogues. *Bulletin of the Chemical Society of Japan*, **2012**, 85, 1244-1244	5.1	
112	Effect of the axial ligand on the reactivity of the oxoiron(IV) porphyrin □-cation radical complex: higher stabilization of the product state relative to the reactant state. *Inorganic Chemistry*, **2012**, 51, 7296-305	5.1	66
111	Accuracy estimations of overtone vibrational transition frequencies of optically trapped 174Yb6Li molecules. *Physical Review A*, **2012**, 85,	2.6	18
110	Nuclear Magnetic Shielding and Aromaticity of [18]Annulene and Its Quasi-M□bius-Type Analogues. *Bulletin of the Chemical Society of Japan*, **2011**, 84, 845-854	5.1	2
109	Relativistic effect on 77Se NMR chemical shifts of various selenium species in the framework of zeroth-order regular approximation. *Journal of Physical Chemistry A*, **2011**, 115, 8721-30	2.8	16
108	Estimated accuracies of pure XH+(X: even isotopes of group II atoms) vibrational transition frequencies: towards the test of the variance inmp/me. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2011**, 44, 025402	1.3	29
107	Ab initio study of permanent electric dipole moment and radiative lifetimes of alkaline-earth-metal--Li molecules. *Physical Review A*, **2011**, 84,	2.6	31
106	Magnetic-field effects in transitions of X Li molecules (X: even isotopes of group II atoms). *Physical Review A*, **2011**, 84,	2.6	11
105	Elimination of the Stark shift from the vibrational transition frequency of optically trapped 174Yb6Li molecules. *Physical Review A*, **2011**, 84,	2.6	37
104	Electronic Excited States Calculated Using Generalized Spin-Orbital Functions Including Spin-Orbit Interactions. *Journal of Computer Chemistry Japan*, **2011**, 10, 11-17	0.2	7
103	Excitation and circular dichroism spectra of (+)-(S,S)-bis(2-methylbutyl)chalcogenides. *Molecules*, **2010**, 15, 2357-73	4.8	3
102	Relativistic calculations of ground and excited states of LiYb molecule for ultracold photoassociation spectroscopy studies. *Journal of Chemical Physics*, **2010**, 133, 124317	3.9	36

101	Magnetic shielding constants calculated by the infinite-order Douglas-Kroll-Hess method with electron-electron relativistic corrections. *Journal of Chemical Physics*, **2010**, 132, 174105	3.9	29
100	Ab initiostudy on vibrational dipole moments of XH+molecular ions: X =24Mg,40Ca,64Zn,88Sr,114Cd,138Ba,174Yb and202Hg. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2010**, 43, 245102	1.3	30
99	Ligand effect on uranium isotope fractionations caused by nuclear volume effects: An ab initio relativistic molecular orbital study. *Journal of Chemical Physics*, **2010**, 133, 044309	3.9	25
98	Dilithioplumbole: a lead-bearing aromatic cyclopentadienyl analog. *Science*, **2010**, 328, 339-42	33.3	95
97	Expectation values in two-component relativistic theories. *Journal of Chemical Physics*, **2010**, 132, 164108	3.9	27
96	Calculations and Electronic Analyses of55Mn and13C Nuclear Magnetic Shielding Constants for Mn(CO)5X (X = H, F, Cl, Br, I, and CH3) and M(CO)(NH3)3(M = Cr2+, Fe2+, Cu+, and Zn2+). *Bulletin of the Chemical Society of Japan*, **2010**, 83, 514-519	5.1	1
95	A Hybrid Data Base: Quantum Chemistry Literature Data Base II—New Concept and New Methodology—*Bulletin of the Chemical Society of Japan*, **2010**, 83, 660-666	5.1	1
94	Unique properties and reactivity of high-valent manganese-oxo versus manganese-hydroxo in the salen platform. *Inorganic Chemistry*, **2010**, 49, 6664-72	5.1	63
93	Effects of ambient pressure on Cu K□X-ray radiation with millijoule and high-repetition-rate femtosecond laser. *Applied Physics B: Lasers and Optics*, **2010**, 99, 173-179	1.9	13
92	Relativistic and electron-correlation effects on magnetizabilities investigated by the Douglas-Kroll-Hess method and the second-order M□ller-Plesset perturbation theory. *Journal of Computational Chemistry*, **2009**, 30, 2550-66	3.5	11
91	Critical role of external axial ligands in chirality amplification of trans-cyclohexane-1,2-diamine in salen complexes. *Journal of the American Chemical Society*, **2009**, 131, 12394-405	16.4	45
90	Effect of a tridentate ligand on the structure, electronic structure, and reactivity of the copper(I) nitrite complex: role of the conserved three-histidine ligand environment of the type-2 copper site in copper-containing nitrite reductases. *Journal of the American Chemical Society*, **2008**, 130, 6088-98	16.4	48
89	An ab initio molecular orbital study of the nuclear volume effects in uranium isotope fractionations. *Journal of Chemical Physics*, **2008**, 129, 164309	3.9	66
88	An ab initio study based on a finite nucleus model for isotope fractionation in the U(III)-U(IV) exchange reaction system. *Journal of Chemical Physics*, **2008**, 128, 144309	3.9	23
87	Evaluation of electron population terms for 4p, 3p, and (2p): how do HOMO and LUMO shrink or expand depending on nuclear charges?. *Chemistry - A European Journal*, **2008**, 14, 7278-84	4.8	5
86	Contributions from atomic p(Se), d(Se), and f(Se) orbitals to absolute paramagnetic shielding tensors in neutral and charged SeHn and some oxides including the effect of methyl and halogen substitutions on sigmap(Se). *Chemistry - A European Journal*, **2008**, 14, 9647-55	4.8	5
85	Excitation and circular dichroism spectra of (-)-(3aS, 7aS)-2-chalcogena-trans-hydrindans(Ch = S, Se, Te): SAC and SAC-CI calculations. *Journal of Computational Chemistry*, **2008**, 29, 612-21	3.5	6
84	Relativistic quantum-chemical calculations of magnetizabilities of noble gas atoms using the Douglas□Kroll□Hess method. *Chemical Physics Letters*, **2008**, 458, 223-226	2.5	10

83	Examination of accuracy of electron–electron Coulomb interactions in two-component relativistic methods. *Chemical Physics Letters*, **2008**, 461, 327-331	2.5	49
82	Ground and excited states of singlet, cation doublet, and anion doublet states of o-benzoquinone: a theoretical study. *Journal of Physical Chemistry A*, **2007**, 111, 2634-9	2.8	16
81	How (77)Se NMR chemical shifts originate from pre-alpha, alpha, beta, and gamma effects: interpretation based on molecular orbital theory. *Chemistry - A European Journal*, **2007**, 13, 5282-93	4.8	12
80	Calculations of frequency-dependent molecular magnetizabilities with quasi-relativistic time-dependent generalized unrestricted Hartree-Fock method. *Journal of Computational Chemistry*, **2007**, 28, 740-7	3.5	11
79	Applicability of the lowest-order two-electron Breit–Pauli relativistic correction in many-electron heavy and super-heavy elements. *Chemical Physics Letters*, **2007**, 442, 134-139	2.5	13
78	Apoptosis and micronuclei induction in human epithelial cells exposed to energetic carbon ions in the Bragg peak region. *Advances in Space Research*, **2007**, 40, 501-505	2.4	3
77	Chromosome aberrations induced by dual exposure of protons and iron ions. *Radiation and Environmental Biophysics*, **2007**, 46, 125-9	2	22
76	Orientational effect of aryl groups on 77Se NMR chemical shifts: experimental and theoretical investigations. *Chemistry - A European Journal*, **2006**, 12, 3829-46	4.8	37
75	Induction of micronuclei in human fibroblasts across the Bragg curve of energetic heavy ions. *Radiation Research*, **2006**, 166, 583-9	3.1	22
74	SAC and SAC-CI calculations of excitation and circular dichroism spectra of straight-chain and cyclic dichalcogens. *Journal of Physical Chemistry A*, **2006**, 110, 10053-62	2.8	18
73	Theoretical studies on magnetic circular dichroism by the finite perturbation method with relativistic corrections. *Journal of Chemical Physics*, **2005**, 123, 164113	3.9	29
72	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	2.5	27
71	GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMILTONIANS. *Recent Advances in Computational*, **2004**, 191-220		
70	Quantum-chemical calculations for paramagnetic 13C NMR chemical shifts of iron-bound cyanide ions of iron porphyrins in ground and low-lying excited states containing ferric (dxy)2(dxz,yz)3 and (dxy)1(dxz,yz)4 configurations. *Journal of the American Chemical Society*, **2004**, 126, 486-7	16.4	13
69	Nuclear Magnetic Shielding Constants of Halogens in X- and XO4-(X = F, Cl, Br, I) – Relativistic and Electron-Correlation Effects –. *Journal of Computer Chemistry Japan*, **2004**, 3, 153-158	0.2	
68	Quasirelativistic theory for magnetic shielding constants. II. Gauge-including atomic orbitals and applications to molecules. *Journal of Chemical Physics*, **2003**, 118, 1027-1035	3.9	95
67	Quasirelativistic theory for the magnetic shielding constant. I. Formulation of Douglas–Kroll–Hess transformation for the magnetic field and its application to atomic systems. *Journal of Chemical Physics*, **2003**, 118, 1015-1026	3.9	100
66	Relativistic effects on magnetic circular dichroism studied by GUHF/SECI method. *Chemical Physics Letters*, **2002**, 355, 219-225	2.5	21

65	Excited and Ionized States of p-Benzoquinone and Its Anion Radical: SAC□I Theoretical Study. *Journal of Physical Chemistry A*, **2002**, 106, 3838-3849	2.8	55
64	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. *Journal of Chemical Physics*, **2002**, 117, 2045-2052	3.9	46
63	Ionized and excited states of ferrocene: Symmetry adapted cluster□onfiguration□nteraction study. *Journal of Chemical Physics*, **2002**, 117, 6533-6537	3.9	30
62	Excited states of four hemes in a c-type cytochrome subunit of the photosynthetic reaction center of Rhodopseudomonas viridis: SAC-CI calculations. *Journal of Porphyrins and Phthalocyanines*, **2001**, 05, 256-266	1.8	9
61	Relativistic effects and the halogen dependencies in the 13C chemical shifts of CH4□In, CH4□Brn, CCl4□In, and CBr4□In (n=0□). *Journal of Computational Chemistry*, **2001**, 22, 528-536	3.5	33
60	Quasirelativistic study of 125Te nuclear magnetic shielding constants and chemical shifts. *Journal of Computational Chemistry*, **2001**, 22, 1502-1508	3.5	24
59	Effect of ion-exchanged alkali metal cations on the photolysis of 2-pentanone included within ZSM-5 zeolite cavities: a study of ab initio molecular orbital calculations. *Research on Chemical Intermediates*, **2001**, 27, 89-102	2.8	3
58	Electronic excitation and ionization spectra of azabenzenes: Pyridine revisited by the symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 5117-5123	3.9	44
57	Electronic excitation spectrum of thiophene studied by symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 842	3.9	49
56	Quasi-Relativistic Study of 199Hg Nuclear Magnetic Shielding Constants of Dimethylmercury, Disilylmercury and Digermylmercury. *Journal of Physical Chemistry A*, **2001**, 105, 128-133	2.8	14
55	Dirac□ock 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	2.5	38
54	Electronic excitation and ionization spectra of cyclopentadiene: Revisit by the symmetry-adapted cluster□onfiguration interaction method. *Journal of Chemical Physics*, **2000**, 113, 5245	3.9	32
53	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster□onfiguration interaction method. *Journal of Chemical Physics*, **2000**, 113, 7853-7866	3.9	82
52	Dirac□ock calculations of magnetic shielding constants: hydrogen molecule and hydrogen halides. *Chemical Physics Letters*, **1999**, 310, 342-346	2.5	28
51	Theoretical study of the decomposition of HCOOH on an MgO(100) surface. *Surface Science*, **1999**, 429, 133-142	1.8	24
50	Relativistic theory of the magnetic shielding constant:. *Chemical Physics Letters*, **1998**, 283, 119-124	2.5	47
49	Theoretical Study on the Decomposition of HCOOH on a ZnO(1010) Surface. *Journal of Catalysis*, **1998**, 173, 53-63	7.3	38
48	Self-Condensation Reaction of Lithium (Alkoxy)silylenoid: A Model Study by ab Initio Calculation. *Organometallics*, **1998**, 17, 4573-4577	3.8	28

47	Theoretical Study of the Excited States of Chlorin, Bacteriochlorin, Pheophytin a, and Chlorophyll a by the SAC/SAC□I Method. *Journal of Physical Chemistry B*, **1998**, 102, 1320-1326	3.4	89
46	Topology of density difference and force analysis. *Theoretica Chimica Acta*, **1996**, 93, 67-78		24
45	The Electronic Spectra of Ethylene. *Bulletin of the Chemical Society of Japan*, **1996**, 69, 1901-1906	5.1	7
44	Theoretical Study on Metal NMR Chemical Shifts. Electronic Mechanism of the Xe Chemical Shift. *Bulletin of the Chemical Society of Japan*, **1996**, 69, 953-959	5.1	18
43	CO and NO adsorption on copper-containing zeolite. A theoretical ab initio study. *Catalysis Letters*, **1996**, 42, 173-176	2.8	27
42	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method. Electronic mechanism in the aluminum compounds, A1X4□(X = H, F, Cl, Br and I). *Chemical Physics Letters*, **1996**, 249, 284-289	2.5	36
41	Ground and excited states of Mg porphin studied by the SAC/SAC-CI method. *Chemical Physics Letters*, **1996**, 250, 159-164	2.5	54
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