Hiroshi Nakatsuji

List of Publications by Citations

140 papers	6,498 citations	44 h-index	76 g-index
144 ext. papers	6,758 ext. citations	4 avg, IF	6.06 L-index

#	Paper	IF	Citations
140	Cluster expansion of the wavefunction. Electron correlations in ground and excited states by SAC (symmetry-adapted-cluster) and SAC CI theories. *Chemical Physics Letters*, **1979**, 67, 329-333	2.5	537
139	Cluster expansion of the wavefunction. Calculation of electron correlations in ground and excited states by SAC and SAC CI theories. *Chemical Physics Letters*, **1979**, 67, 334-342	2.5	304
138	Cluster expansion of the wavefunction, valence and rydberg excitations, ionizations, and inner-valence ionizations of CO2 and N2O studied by the sac and sac CI theories. *Chemical Physics*, **1983**, 75, 425-441	2.3	255
137	Direct determination of the quantum-mechanical density matrix using the density equation. *Physical Review Letters*, **1996**, 76, 1039-1042	7.4	237
136	Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm. *Journal of Chemical Physics*, **2001**, 114, 8282-8292	3.9	217
135	Equation for the direct determination of the density matrix. *Physical Review A*, **1976**, 14, 41-50	2.6	216
134	Description of two- and many-electron processes by the SAC-CI method. *Chemical Physics Letters*, **1991**, 177, 331-337	2.5	177
133	Excited and ionized states of free base porphin studied by the symmetry adapted cluster-configuration interaction (SAC-CI) method. *Journal of Chemical Physics*, **1996**, 104, 2321-2329	3.9	157
132	Solving the Schrodinger equation for helium atom and its isoelectronic ions with the free iterative complement interaction (ICI) method. *Journal of Chemical Physics*, **2007**, 127, 224104	3.9	130
131	Theoretical Studies on the Color-Tuning Mechanism in Retinal Proteins. *Journal of Chemical Theory and Computation*, **2007**, 3, 605-18	6.4	122
130	Red light in chemiluminescence and yellow-green light in bioluminescence: color-tuning mechanism of firefly, Photinus pyralis, studied by the symmetry-adapted cluster-configuration interaction method. *Journal of the American Chemical Society*, **2007**, 129, 8756-65	16.4	118
129	Structure of the exact wave function. *Journal of Chemical Physics*, **2000**, 113, 2949-2956	3.9	104
128	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
127	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
126	Scaled Schr□dinger equation and the exact wave function. *Physical Review Letters*, **2004**, 93, 030403	7.4	89
125	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster□configuration interaction method. *Journal of Chemical Physics*, **2000**, 113, 7853-7866	3.9	82
124	SAC-CI Method: Theoretical Aspects and Some Recent Topics. *Computational Chemistry - Reviews of Current Trends*, **1997**, 62-124		80

123	Formulation and implementation of direct algorithm for the symmetry-adapted cluster and symmetry-adapted cluster-configuration interaction method. *Journal of Chemical Physics*, **2008**, 128, 094105	3.9	80
122	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-CI study. *Journal of Computational Chemistry*, **2003**, 24, 1421-31	3.5	78
121	Density matrix variational theory: Application to the potential energy surfaces and strongly correlated systems. *Journal of Chemical Physics*, **2002**, 116, 5432-5439	3.9	78
120	Excited states of GFP chromophore and active site studied by the SAC-CI method: effect of protein-environment and mutations. *Journal of Computational Chemistry*, **2007**, 28, 2443-52	3.5	76
119	Electrostatic force theory for a molecule and interacting molecules. I. Concept and illustrative applications. *Journal of the American Chemical Society*, **1973**, 95, 345-354	16.4	76
118	Ab initio molecular orbital model of scanning tunneling microscopy. *Journal of Chemical Physics*, **1996**, 104, 2410-2417	3.9	74
117	Multireference cluster expansion theory: MRSAC theory. *Journal of Chemical Physics*, **1985**, 83, 713-722	3.9	72
116	Cluster expansion of the wave function. Valence and Rydberg excitations and ionizations of ethylene. *Journal of Chemical Physics*, **1984**, 80, 3703-3709	3.9	69
115	Excited States of Free Base Phthalocyanine Studied by the SAC-CI Method. *Journal of Physical Chemistry A*, **1997**, 101, 446-451	2.8	67
114	Dipped adcluster model study for molecular and dissociative chemisorptions of O2 on Ag surface. *Journal of Chemical Physics*, **1993**, 98, 2423-2436	3.9	67
113	Analytical energy gradient of the ground, excited, ionized and electron-attached states calculated by the SAC/SAC-CI method. *Chemical Physics Letters*, **1997**, 280, 79-84	2.5	66
112	Mechanism of color tuning in retinal protein: SAC-CI and QM/MM study. *Chemical Physics Letters*, **2005**, 414, 239-242	2.5	66
111	Cluster expansion of the wave function. Electron correlations in singlet and triplet excited states, ionized states, and electron attached states by SAC and SACCI theories. *International Journal of Quantum Chemistry*, **1981**, 20, 1301-1313	2.1	65
110	Exponentially generated configuration interaction theory. Descriptions of excited, ionized, and electron attached states. *Journal of Chemical Physics*, **1991**, 94, 6716-6727	3.9	64
109	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface. *Journal of Chemical Physics*, **1987**, 87, 4995-5001	3.9	62
108	Exponentially generated wave functions. *Journal of Chemical Physics*, **1985**, 83, 5743-5748	3.9	61
107	Helical structure and circular dichroism spectra of DNA: a theoretical study. *Journal of Physical Chemistry A*, **2013**, 117, 42-55	2.8	59
106	Structure of the exact wave function. II. Iterative configuration interaction method. *Journal of Chemical Physics*, **2001**, 115, 2000-2006	3.9	56

105	Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SAC□I (configuration interaction) method. *Chemical Physics*, **1999**, 242, 177-193	2.3	56
104	On the Unrestricted Hartree□ock Wavefunction. *Journal of Chemical Physics*, **1969**, 51, 3175-3180	3.9	55
103	Theoretical study on the ground and excited states of MnO_4^-. *Journal of Chemical Physics*, **1991**, 95, 8287-8291	3.9	53
102	Analytically solving the relativistic Dirac-Coulomb equation for atoms and molecules. *Physical Review Letters*, **2005**, 95, 050407	7.4	50
101	Mechanism of methanol synthesis on Cu(100) and Zn/Cu(100) surfaces: Comparative dipped adcluster model study. *International Journal of Quantum Chemistry*, **2000**, 77, 341-349	2.1	50
100	Deepening and Extending the Quantum Principles in Chemistry. *Bulletin of the Chemical Society of Japan*, **2005**, 78, 1705-1724	5.1	49
99	A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. *Organometallics*, **2008**, 27, 1736-1742	3.8	47
98	General method of solving the Schr□inger equation of atoms and molecules. *Physical Review A*, **2005**, 72,	2.6	47
97	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. *Journal of Chemical Physics*, **2002**, 117, 2045-2052	3.9	46
96	Solving non-Born-Oppenheimer Schr□inger equation for hydrogen molecular ion and its isotopomers using the free complement method. *Journal of Chemical Physics*, **2009**, 130, 024102	3.9	44
95	Origin of color tuning in human red, green, and blue cone pigments: SAC-CI and QM/MM study. *Chemical Physics Letters*, **2008**, 462, 318-320	2.5	44
94	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
93	Free iterative-complement-interaction calculations of the hydrogen molecule. *Physical Review A*, **2005**, 72,	2.6	43
92	Symmetry-adapted cluster□onfiguration interaction method applied to high-spin multiplicity. *Journal of Chemical Physics*, **1993**, 98, 7179-7184	3.9	43
91	Solving the Schr□inger equation of helium and its isoelectronic ions with the exponential integral (Ei) function in the free iterative complement interaction method. *Physical Chemistry Chemical Physics*, **2008**, 10, 4486-94	3.6	40
90	Structure of the exact wave function. III. Exponential ansatz. *Journal of Chemical Physics*, **2001**, 115, 2465-2475	3.9	40
89	Discovery of a general method of solving the Schr□inger and dirac equations that opens a way to accurately predictive quantum chemistry. *Accounts of Chemical Research*, **2012**, 45, 1480-90	24.3	39
88	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface: Image force correction and applications to Pd□2 adclusters. *Journal of Chemical Physics*, **1991**, 95, 640-647	3.9	38

87	Iterative Cl general singles and doubles (ICIGSD) method for calculating the exact wave functions of the ground and excited states of molecules. *Journal of Chemical Physics*, **2005**, 122, 194108	3.9	37
86	On the color-tuning mechanism of Human-Blue visual pigment: SAC-CI and QM/MM study. *Chemical Physics Letters*, **2006**, 432, 252-256	2.5	36
85	Analytical energy gradients of the excited, ionized and electron-attached states calculated by the SAC-CI general-R method. *Chemical Physics Letters*, **2001**, 347, 493-498	2.5	36
84	Structure of the exact wave function. V. Iterative configuration interaction method for molecular systems within finite basis. *Journal of Chemical Physics*, **2002**, 117, 9-12	3.9	36
83	Artificial color tuning of firefly luminescence: Theoretical mutation by tuning electrostatic interactions between protein and luciferin. *Chemical Physics Letters*, **2009**, 469, 191-194	2.5	35
82	Color Tuning Mechanism of Human Red, Green, and Blue Cone Pigments: SAC-CI Theoretical Study. *Bulletin of the Chemical Society of Japan*, **2009**, 82, 1140-1148	5.1	34
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76	Peralkylated Tetrasilanes:□Conformational Dependence of the Photoelectron Spectrum□ *Journal of Physical Chemistry A*, **2002**, 106, 2369-2373	2.8	32
75	How accurately does the free complement wave function of a helium atom satisfy the Schrödinger equation?. *Physical Review Letters*, **2008**, 101, 240406	7.4	31
74	Fine theoretical spectroscopy using symmetry adapted cluster-configuration interaction general-R method: Outer- and inner-valence ionization spectra of CS2 and OCS. *Journal of Chemical Physics*, **2002**, 117, 3248-3255	3.9	31
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72	SAC-CI GENERAL-R METHOD: THEORY AND APPLICATIONS TO THE MULTI-ELECTRON PROCESSES **2002**, 293-319		31
71	Direct determination of second-order density matrix using density equation: Open-shell system and excited state. *Journal of Chemical Physics*, **2000**, 112, 8772-8778	3.9	31
70	Inverse Schrödinger equation and the exact wave function. *Physical Review A*, **2002**, 65,	2.6	30

69	Ionized and excited states of ferrocene: Symmetry adapted cluster□configuration□interaction study. *Journal of Chemical Physics*, **2002**, 117, 6533-6537	3.9	30
68	Self-Condensation Reaction of Lithium (Alkoxy)silylenoid: A Model Study by ab Initio Calculation. *Organometallics*, **1998**, 17, 4573-4577	3.8	28
67	Potential energy curves of the ground, excited, and ionized states of Ar2 studied by the symmetry adapted cluster-configuration interaction theory. *Journal of Chemical Physics*, **1990**, 92, 6084-6092	3.9	28
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65	Electronic mechanism of the surface enhanced Raman scattering. *Journal of Chemical Physics*, **1995**, 103, 2286-2294	3.9	26
64	Hyperfine splitting constants studied by the symmetry adapted cluster-configuration interaction method. *Journal of Chemical Physics*, **1994**, 100, 5821-5828	3.9	25
63	Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. *International Journal of Quantum Chemistry*, **1997**, 65, 839-855	2.1	24
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61	Solving the Schr□dinger and Dirac equations of hydrogen molecular ion accurately by the free iterative complement interaction method. *Journal of Chemical Physics*, **2008**, 128, 124103	3.9	23
60	Theoretical study for the excited states of MoO_4^{n-} and MoS_2□ (n=0~4) and $MoSe_2$□. *Journal of Chemical Physics*, **1990**, 93, 1865-1875	3.9	23
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54	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
53	Mixed-exponentially generated wave function method for ground, excited, ionized, and electron attached states of a molecule. *Journal of Chemical Physics*, **1991**, 95, 4296-4305	3.9	18
52	Free-complement local-Schr□dinger-equation method for solving the Schr□dinger equation of atoms and molecules: basic theories and features. *Journal of Chemical Physics*, **2015**, 142, 084117	3.9	17

51	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis: Theoretical Study. *Journal of Physical Chemistry B*, **2003**, 107, 838-847	3.4	17
50	Similarities and Differences between RNA and DNA Double-Helical Structures in Circular Dichroism Spectroscopy: A SAC-CI Study. *Journal of Physical Chemistry A*, **2016**, 120, 9008-9018	2.8	15
49	Theoretical investigation on the valence ionization spectra of Cl2O, ClOOCl, and F2O by correlation-based configuration interaction methods. *Journal of Chemical Physics*, **2003**, 118, 5811-5820	3.9	15
48	CASSCF study of bonding in NiCO and FeCO. *International Journal of Quantum Chemistry*, **1999**, 72, 221-231	2.1	15
47	Indicator of the Stacking Interaction in the DNA Double-Helical Structure: ChiraSac Study. *Journal of Physical Chemistry A*, **2015**, 119, 8269-78	2.8	14
46	Conformational dependence of the circular dichroism spectrum of □-hydroxyphenylacetic acid: a ChiraSac study. *Journal of Physical Chemistry A*, **2013**, 117, 14065-74	2.8	14
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44	Circular Dichroism and Absorption Spectroscopy for Three-Membered Ring Compounds Using Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI) Method. *Bulletin of the Chemical Society of Japan*, **2009**, 82, 1215-1226	5.1	14
43	General coalescence conditions for the exact wave functions: higher-order relations for two-particle systems. *Journal of Chemical Physics*, **2013**, 139, 044114	3.9	13
42	SOLVING THE NON-BORN-OPPENHEIMER SCHR□DINGER EQUATION FOR THE HYDROGEN MOLECULAR ION WITH THE FREE COMPLEMENT METHOD. II. HIGHLY ACCURATE ELECTRONIC, VIBRATIONAL, AND ROTATIONAL EXCITED STATES. *Astrophysical Journal*, **2013**, 770, 144	4.7	13
41	How does the free complement wave function become accurate and exact finally for the hydrogen atom starting from the Slater and Gaussian initial functions and for the helium atom on the cusp conditions?. *International Journal of Quantum Chemistry*, **2009**, 109, 2248-2262	2.1	12
40	Electronic circular dichroism spectrum of uridine studied by the SAC□CI method. *Chemical Physics Letters*, **2006**, 425, 367-371	2.5	12
39	Roles of proteins in the electron transfer in the photosynthetic reaction center of Rhodopseudomonas viridis: bacteriopheophytin to ubiquinone. *Journal of Computational Chemistry*, **2001**, 22, 265-272	3.5	12
38	Theoretical model studies for surface-molecule interacting systems. *International Journal of Quantum Chemistry*, **1992**, 44, 725-736	2.1	12
37	Solving the Schr□dinger equation of atoms and molecules with the free-complement chemical-formula theory: First-row atoms and small molecules. *Journal of Chemical Physics*, **2018**, 149, 114106	3.9	12
36	Circular dichroism spectra of uridine derivatives: ChiraSac study. *Journal of Physical Chemistry A*, **2014**, 118, 2931-41	2.8	11
35	Analytical evaluations of exponentially correlated unlinked one-center, three- and four-electron integrals. *Physical Review A*, **2012**, 85,	2.6	11
34	Equation for the direct determination of the density matrix: Time-dependent density equation and perturbation theory. *Theoretical Chemistry Accounts*, **1999**, 102, 97-104	1.9	11

33	Exponentially generated configuration interaction (EGCI) method applied to high-spin multiplicity. *Journal of Chemical Physics*, **1993**, 99, 1952-1961	3.9	11
32	The Hellmann-Feynman theorem applied to long-range forces. *Theoretica Chimica Acta*, **1976**, 41, 119-131		11
31	Solving the Schrödinger equation of molecules by relaxing the antisymmetry rule: Inter-exchange theory. *Journal of Chemical Physics*, **2015**, 142, 194101	3.9	10
30	Excited-state geometries and vibrational frequencies studied using the analytical energy gradients of the direct symmetry-adapted cluster-configuration interaction method. I. HAX-type molecules. *Journal of Chemical Physics*, **2011**, 135, 044316	3.9	10
29	Solving the Schrödinger equation of atoms and molecules: Chemical-formula theory, free-complement chemical-formula theory, and intermediate variational theory. *Journal of Chemical Physics*, **2018**, 149, 114105	3.9	10
28	Electronic excitation spectra of doublet anion radicals of cyanobenzene and nitrobenzene derivatives: SAC-CI theoretical studies This paper is dedicated to the Late Professor Nicholas Charles Handy for his fundamental achievements in the field of molecular	1.7	9
27	Exploring Photobiology and Biospectroscopy with the Sac-Ci (Symmetry-Adapted Cluster-Configuration Interaction) Method. *Challenges and Advances in Computational Chemistry and Physics*, **2008**, 93-124	0.7	9
26	Solving the Schrödinger equation with the free-complement chemical-formula theory: Variational study of the ground and excited states of Be and Li atoms. *Journal of Chemical Physics*, **2019**, 150, 044105	3.9	8
25	Solving the Schrödinger equation of hydrogen molecules with the free-complement variational theory: essentially exact potential curves and vibrational levels of the ground and excited states of the symmetry. *Physical Chemistry Chemical Physics*, **2019**, 21, 6327-6340	3.6	8
24	Ferromagnetic Interaction in Organic Radical Ion Salts. *Molecular Crystals and Liquid Crystals*, **1993**, 232, 117-134		8
23	Efficient antisymmetrization algorithm for the partially correlated wave functions in the free complement-local Schrödinger equation method. *Journal of Chemical Physics*, **2013**, 139, 044112	3.9	7
22	Electron transfer in the c-type cytochrome subunit of the photosynthetic reaction center of Rhodopseudomonas viridis: ab initio theoretical study. *Journal of Computational Chemistry*, **2001**, 22, 521-527	3.5	7
21	Light-Driven Proton, Sodium Ion, and Chloride Ion Transfer Mechanisms in Rhodopsins: SAC-CI Study. *Journal of Physical Chemistry A*, **2019**, 123, 1766-1784	2.8	7
20	Solving the Schrödinger equation of atoms and molecules using one- and two-electron integrals only. *Physical Review A*, **2020**, 101,	2.6	5
19	Theoretical Surface Spectroscopy of NO on the Pt(111) Surface with the DAM (Dipped Adcluster Model) and the SAC-CI (Symmetry-Adapted-Cluster Configuration-Interaction) Method. *Journal of Chemical Theory and Computation*, **2005**, 1, 239-47	6.4	5
18	Valence ionization spectra of 4 electron molecules with low-lying satellites involving n and transitions. *Molecular Physics*, **2006**, 104, 971-982	1.7	5
17	Magnetic Properties in Charge-Transfer Complexes of High-Symmetry Organic Acceptors. *Materials Research Society Symposia Proceedings*, **1992**, 247, 417		5
16	Hidden potentials in classical theorems. *Journal of Chemical Physics*, **1977**, 67, 1312-1318	3.9	5

15	Accuracy of Td-DFT in the Ultraviolet and Circular Dichroism Spectra of Deoxyguanosine and Uridine. *Journal of Physical Chemistry A*, **2018**, 122, 100-118	2.8	5
14	SPC cluster modeling of metal oxides: ways of determining the values of point charges in the embedded cluster model. *Science in China Series B: Chemistry*, **1998**, 41, 113-121		4
13	Solving the Schr□inger equation of hydrogen molecule with the free complement-local Schr□inger equation method: Potential energy curves of the ground and singly excited singlet and triplet states, □□, □and □*Journal of Chemical Physics*, **2018**, 149, 244116	3.9	4
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11	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
10	Free complement sij-assisted rij theory: Variational calculation of the quintet state of a carbon atom. *Physical Review A*, **2020**, 102,	2.6	3
9	Solving the Schr□inger equation of the hydrogen molecule with the free-complement variational theory: essentially exact potential curves and vibrational levels of the ground and excited states of □symmetry. *Physical Chemistry Chemical Physics*, **2020**, 22, 13489-13497	3.6	2
8	Cluster expansion of the wave function. Ionization and excitation spectra of no radical studied by the SAC and SAC-CI theory. *International Journal of Quantum Chemistry*, **2009**, 24, 241-255	2.1	1
7	Accurate scaling functions of the scaled Schr□inger equation.. *Journal of Chemical Physics*, **2022**, 156, 014113	3.9	1
6	Electronic Theory of the Chemisorption and Catalytic Reactions on Metal Surface.. *Hyomen Kagaku*, **1993**, 14, 603-609		1
5	Photoelectron spectrum of NO : SAC-CI gradient study of vibrational-rotational structures. *Journal of Computational Chemistry*, **2019**, 40, 360-374	3.5	1
4	Circular Dichroism Spectroscopy with the SAC-CI Methodology: A ChiraSac Study **2018**, 21-47		1
3	CASSCF study of bonding in NiCO and FeCO **1999**, 72, 221		1
2	Keiji Morokuma. *Journal of Physical Chemistry A*, **2018**, 122, 880-881	2.8	
1	GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMILTONIANS. *Recent Advances in Computational*, **2004**, 191-220		