

Hiroshi Nakatsuji

List of Publications by Year in descending order

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144
papers

7,020
citations

50276

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80
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144
all docs

144
docs citations

144
times ranked

3119
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate scaling functions of the scaled Schrödinger equation. Journal of Chemical Physics, 2022, 156, 014113.	3.0	6
2	Free complement $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi}s \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi}i \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mi}j \rangle$ -assisted $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi}r \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi}i \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mi}j \rangle$ theory: Variational calculation of the quintet state of a carbon atom. Physical Review A, 2020, 102, .	2.5	5
3	Solving the Schrödinger 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 \hat{I} symmetry. Physical Chemistry Chemical Physics, 2020, 22, 13489-13497.	2.8	3
4	Solving the Schrödinger equation of atoms and molecules using one- and two-electron integrals only. Physical Review A, 2020, 101, .	2.5	10
5	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.	3.0	10
6	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 $\hat{I}\Sigma$ symmetry. Physical Chemistry Chemical Physics, 2019, 21, 6327-6340.	2.8	13
7	Light-Driven Proton, Sodium Ion, and Chloride Ion Transfer Mechanisms in Rhodopsins: SAC-CI Study. Journal of Physical Chemistry A, 2019, 123, 1766-1784.	2.5	8
8	Photoelectron spectrum of $\text{NO}_2^{\hat{a}^-}$: SAC-CI gradient study of vibrational-rotational structures. Journal of Computational Chemistry, 2019, 40, 360-374.	3.3	1
9	Keiji Morokuma. Journal of Physical Chemistry A, 2018, 122, 880-881.	2.5	0
10	Accuracy of Td-DFT in the Ultraviolet and Circular Dichroism Spectra of Deoxyguanosine and Uridine. Journal of Physical Chemistry A, 2018, 122, 100-118.	2.5	9
11	Circular Dichroism Spectroscopy with the SAC-CI Methodology: A ChiraSac Study. , 2018, , 21-47.		1
12	Solving the Schrödinger equation of hydrogen molecule with the free complement "local Schrödinger equation method: Potential energy curves of the ground and singly excited singlet and triplet states, $\hat{I}\Sigma$, $\hat{I}\Pi$, and $\hat{I}\Delta$ ". Journal of Chemical Physics, 2018, 149, 244116.	3.0	8
13	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.	3.0	16
14	Solving the Schrödinger 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.	3.0	15
15	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.	2.5	26
16	Electronic excitation spectra of doublet anion radicals of cyanobenzene and nitrobenzene derivatives: SAC-CI theoretical studies. Molecular Physics, 2015, 113, 1728-1739.	1.7	12
17	Solving the Schrödinger equation of molecules by relaxing the antisymmetry rule: Inter-exchange theory. Journal of Chemical Physics, 2015, 142, 194101.	3.0	12
18	Indicator of the Stacking Interaction in the DNA Double-Helical Structure: ChiraSac Study. Journal of Physical Chemistry A, 2015, 119, 8269-8278.	2.5	15

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19	Free-complement local-Schrödinger-equation method for solving the Schrödinger equation of atoms and molecules: Basic theories and features. <i>Journal of Chemical Physics</i> , 2015, 142, 084117.	3.0	20
20	Circular Dichroism Spectra of Uridine Derivatives: ChiraSac Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2931-2941.	2.5	14
21	General coalescence conditions for the exact wave functions: Higher-order relations for two-particle systems. <i>Journal of Chemical Physics</i> , 2013, 139, 044114.	3.0	15
22	Helical Structure and Circular Dichroism Spectra of DNA: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 42-55.	2.5	77
23	Conformational Dependence of the Circular Dichroism Spectrum of $\hat{\pm}$ -Hydroxyphenylacetic Acid: A ChiraSac Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14065-14074.	2.5	14
24	Non-Born-Oppenheimer potential energy curve: Hydrogen molecular ion with highly accurate free complement method. <i>Journal of Chemical Physics</i> , 2013, 139, 074105.	3.0	15
25	SOLVING THE NON-BORN-OPPENHEIMER SCHRÖDINGER EQUATION FOR THE HYDROGEN MOLECULAR ION WITH THE FREE COMPLEMENT METHOD. II. HIGHLY ACCURATE ELECTRONIC, VIBRATIONAL, AND ROTATIONAL EXCITED STATES. <i>Astrophysical Journal</i> , 2013, 770, 144.	4.5	15
26	Efficient antisymmetrization algorithm for the partially correlated wave functions in the free complement-local Schrödinger equation method. <i>Journal of Chemical Physics</i> , 2013, 139, 044112.	3.0	7
27	Analytical evaluations of exponentially correlated unlinked one-center, three- and four-electron integrals. <i>Physical Review A</i> , 2012, 85, .	2.5	13
28	Electronic structure and optical properties of conjugated molecules: SAC-CI study. , 2012, , .		0
29	Accurate solutions of the Schrödinger and Dirac equations of H^+ , HD^+ , and HT^+ : With and without Born-Oppenheimer approximation and under magnetic field. <i>Chemical Physics</i> , 2012, 401, 62-72.	1.9	26
30	Discovery of a General Method of Solving the Schrödinger and Dirac Equations That Opens a Way to Accurately Predictive Quantum Chemistry. <i>Accounts of Chemical Research</i> , 2012, 45, 1480-1490.	15.6	53
31	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. <i>Journal of Chemical Physics</i> , 2011, 135, 044316.	3.0	10
32	LiH potential energy curves for ground and excited states with the free complement local Schrödinger equation method. <i>Chemical Physics Letters</i> , 2010, 496, 347-350.	2.6	29
33	SOLVING THE SCHRÖDINGER AND DIRAC EQUATIONS FOR A HYDROGEN ATOM IN THE UNIVERSE'S STRONGEST MAGNETIC FIELDS WITH THE FREE COMPLEMENT METHOD. <i>Astrophysical Journal</i> , 2010, 725, 528-533.	4.5	19
34	Solving non-Born-Oppenheimer Schrödinger equation for hydrogen molecular ion and its isotopomers using the free complement method. <i>Journal of Chemical Physics</i> , 2009, 130, 024102.	3.0	45
35	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?. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2248-2262.	2.0	12
36	Artificial color tuning of firefly luminescence: Theoretical mutation by tuning electrostatic interactions between protein and luciferin. <i>Chemical Physics Letters</i> , 2009, 469, 191-194.	2.6	39

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37	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.	3.2	16
38	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.	3.2	35
39	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.	2.6	46
40	Solving the Schrödinger 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.	2.8	42
41	A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. Organometallics, 2008, 27, 1736-1742.	2.3	47
42	Exploring Photobiology and Biospectroscopy with the Sac-Ci (Symmetry-Adapted) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 Td (Cluster and Physics, 2008, , 93-124.	0.6	9
43	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.	3.0	84
44	Photochemistry of Biological Chemosensors, Organic Light-Emitting Diodes, and Inner-shell Electronic Processes. AIP Conference Proceedings, 2008, , .	0.4	0
45	Solving the Schrödinger and Dirac equations of hydrogen molecular ion accurately by the free iterative complement interaction method. Journal of Chemical Physics, 2008, 128, 124103.	3.0	28
46	How Accurately Does the Free Complement Wave Function of a Helium Atom Satisfy the Schrödinger Equation?. Physical Review Letters, 2008, 101, 240406.	7.8	35
47	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
48	Solving the Schrödinger equation for helium atom and its isoelectronic ions with the free iterative complement interaction (ICI) method. Journal of Chemical Physics, 2007, 127, 224104.	3.0	142
49	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, 8756-8765.	13.7	127
50	Theoretical Studies on the Color-Tuning Mechanism in Retinal Proteins. Journal of Chemical Theory and Computation, 2007, 3, 605-618.	5.3	134
51	Photochemistry of Organic Light-Emitting Diodes. AIP Conference Proceedings, 2007, , .	0.4	0
52	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, 2443-2452.	3.3	78
53	Valence ionization spectra of 4f-electron molecules with low-lying satellites involving π^* and π^* transitions. Molecular Physics, 2006, 104, 971-982.	1.7	5
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, 10053-10062.	2.5	19

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55	Electronic circular dichroism spectrum of uridine studied by the SAC-Cl method. Chemical Physics Letters, 2006, 425, 367-371.	2.6	12
56	On the color-tuning mechanism of Human-Blue visual pigment: SAC-Cl and QM/MM study. Chemical Physics Letters, 2006, 432, 252-256.	2.6	36
57	Deepening and Extending the Quantum Principles in Chemistry. Bulletin of the Chemical Society of Japan, 2005, 78, 1705-1724.	3.2	51
58	Mechanism of color tuning in retinal protein: SAC-Cl and QM/MM study. Chemical Physics Letters, 2005, 414, 239-242.	2.6	67
59	Analytically Solving the Relativistic Dirac-Coulomb Equation for Atoms and Molecules. Physical Review Letters, 2005, 95, 050407.	7.8	54
60	Iterative CI 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.	3.0	37
61	General method of solving the Schrödinger equation of atoms and molecules. Physical Review A, 2005, 72, .	2.5	51
62	Theoretical Surface Spectroscopy of NO on the Pt(111) Surface with the DAM (Dipped Adcluster Model) and the SAC-Cl (Symmetry-Adapted-Cluster Configuration-Interaction) Method. Journal of Chemical Theory and Computation, 2005, 1, 239-247.	5.3	5
63	Free iterative-complement-interaction calculations of the hydrogen molecule. Physical Review A, 2005, 72, .	2.5	45
64	Analytical energy gradient of the symmetry-adapted-cluster configuration-interaction general-R method for singlet to septet ground and excited states. Journal of Chemical Physics, 2004, 120, 2593-2605.	3.0	34
65	GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMILTONIANS. Recent Advances in Computational, 2004, , 191-220.	0.8	0
66	Scaled Schrödinger Equation and the Exact Wave Function. Physical Review Letters, 2004, 93, 030403.	7.8	96
67	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-Cl study. Journal of Computational Chemistry, 2003, 24, 1421-1431.	3.3	83
68	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodospseudomonas Viridis: Theoretical Study. Journal of Physical Chemistry B, 2003, 107, 838-847.	2.6	19
69	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
70	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.	3.0	108
71	Theoretical investigation on the valence ionization spectra of Cl ₂ O, ClOOCl, and F ₂ O by correlation-based configuration interaction methods. Journal of Chemical Physics, 2003, 118, 5811-5820.	3.0	16
72	STRUCTURE OF THE EXACT WAVE FUNCTION: PROGRESS REPORT. , 2003, , .		0

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73	Density matrix variational theory: Application to the potential energy surfaces and strongly correlated systems. <i>Journal of Chemical Physics</i> , 2002, 116, 5432-5439.	3.0	79
74	Inverse Schrödinger equation and the exact wave function. <i>Physical Review A</i> , 2002, 65, .	2.5	38
75	Fine theoretical spectroscopy using symmetry adapted cluster-configuration interaction general-R method: Outer- and inner-valence ionization spectra of CS ₂ and OCS. <i>Journal of Chemical Physics</i> , 2002, 117, 3248-3255.	3.0	32
76	Structure of the exact wave function. IV. Excited states from exponential ansatz and comparative calculations by the iterative configuration interaction and extended coupled cluster theories. <i>Journal of Chemical Physics</i> , 2002, 116, 1811-1824.	3.0	31
77	SAC-CI GENERAL-R METHOD: THEORY AND APPLICATIONS TO THE MULTI-ELECTRON PROCESSES. , 2002, , 293-319.		33
78	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. <i>Journal of Chemical Physics</i> , 2002, 117, 2045-2052.	3.0	52
79	Ionized and excited states of ferrocene: Symmetry adapted cluster-configuration interaction study. <i>Journal of Chemical Physics</i> , 2002, 117, 6533-6537.	3.0	37
80	Structure of the exact wave function. V. Iterative configuration interaction method for molecular systems within finite basis. <i>Journal of Chemical Physics</i> , 2002, 117, 9-12.	3.0	37
81	Peralkylated Tetrasilanes: Conformational Dependence of the Photoelectron Spectrum. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2369-2373.	2.5	33
82	Outer- and inner-valence ionization spectra of NH ₃ , PH ₃ , and AsH ₃ : symmetry-adapted cluster configuration interaction general-R study. <i>Journal of Chemical Physics</i> , 2002, 116, 1934-1943.	3.0	20
83	Electronic excitation and ionization spectra of azabenzene: Pyridine revisited by the symmetry-adapted cluster configuration interaction method. <i>Journal of Chemical Physics</i> , 2001, 114, 5117-5123.	3.0	46
84	Structure of the exact wave function. II. Iterative configuration interaction method. <i>Journal of Chemical Physics</i> , 2001, 115, 2000-2006.	3.0	59
85	Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm. <i>Journal of Chemical Physics</i> , 2001, 114, 8282-8292.	3.0	239
86	Structure of the exact wave function. III. Exponential ansatz. <i>Journal of Chemical Physics</i> , 2001, 115, 2465-2475.	3.0	43
87	Roles of proteins in the electron transfer in the photosynthetic reaction center of <i>Rhodospseudomonas viridis</i> : bacteriopheophytin to ubiquinone. <i>Journal of Computational Chemistry</i> , 2001, 22, 265-272.	3.3	16
88	Electron transfer in the c-type cytochrome subunit of the photosynthetic reaction center of <i>Rhodospseudomonas viridis</i> : ab initio theoretical study. <i>Journal of Computational Chemistry</i> , 2001, 22, 521-527.	3.3	8
89	Relativistic effects and the halogen dependencies in the ¹³ C chemical shifts of CH ₄ ⁿ In, CH ₄ ⁿ Br _n , CCl ₄ ⁿ In, and CBr ₄ ⁿ In (n=0-4). <i>Journal of Computational Chemistry</i> , 2001, 22, 528-536.	3.3	36
90	Quasirelativistic study of ¹²⁵ Te nuclear magnetic shielding constants and chemical shifts. <i>Journal of Computational Chemistry</i> , 2001, 22, 1502-1508.	3.3	25

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91	Analytical energy gradients of the excited, ionized and electron-attached states calculated by the SAC-CI general-R method. <i>Chemical Physics Letters</i> , 2001, 347, 493-498.	2.6	37
92	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. <i>Research on Chemical Intermediates</i> , 2001, 27, 89-102.	2.7	6
93	Mechanism of methanol synthesis on Cu(100) and Zn/Cu(100) surfaces: Comparative dipped adcluster model study. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 341-349.	2.0	55
94	Direct determination of second-order density matrix using density equation: Open-shell system and excited state. <i>Journal of Chemical Physics</i> , 2000, 112, 8772-8778.	3.0	32
95	Structure of the exact wave function. <i>Journal of Chemical Physics</i> , 2000, 113, 2949-2956.	3.0	117
96	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster configuration interaction method. <i>Journal of Chemical Physics</i> , 2000, 113, 7853-7866.	3.0	88
97	Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SAC-CI (configuration interaction) method. <i>Chemical Physics</i> , 1999, 242, 177-193.	1.9	57
98	Equation for the direct determination of the density matrix: Time-dependent density equation and perturbation theory. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 97-104.	1.4	12
99	CASSCF study of bonding in NiCO and FeCO. <i>International Journal of Quantum Chemistry</i> , 1999, 72, 221-231.	2.0	15
100	CASSCF study of bonding in NiCO and FeCO. <i>International Journal of Quantum Chemistry</i> , 1999, 72, 221-231.	2.0	1
101	SPC cluster modeling of metal oxides: ways of determining the values of point charges in the embedded cluster model. <i>Science in China Series B: Chemistry</i> , 1998, 41, 113-121.	0.8	4
102	Self-Condensation Reaction of Lithium (Alkoxy)silylenoid: A Model Study by ab Initio Calculation. <i>Organometallics</i> , 1998, 17, 4573-4577.	2.3	35
103	SAC-CI Method: Theoretical Aspects and Some Recent Topics. <i>Computational Chemistry - Reviews of Current Trends</i> , 1997, , 62-124.	0.4	86
104	Theoretical Study on the Thermal and Photochemical Isomerization Reactions of Dicyanoacetylene Complex of Platinum Pt(PH ₃) ₂ (C ₄ N ₂). <i>Journal of Physical Chemistry A</i> , 1997, 101, 973-980.	2.5	3
105	Excited States of Free Base Phthalocyanine Studied by the SAC-CI Method. <i>Journal of Physical Chemistry A</i> , 1997, 101, 446-451.	2.5	72
106	Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 839-855.	2.0	24
107	Analytical energy gradient of the ground, excited, ionized and electron-attached states calculated by the SAC/SAC-CI method. <i>Chemical Physics Letters</i> , 1997, 280, 79-84.	2.6	66
108	Ab initio molecular orbital model of scanning tunneling microscopy. <i>Journal of Chemical Physics</i> , 1996, 104, 2410-2417.	3.0	80

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109	Excited and ionized states of free base porphyrin studied by the symmetry adapted cluster configuration interaction (SAC-CI) method. Journal of Chemical Physics, 1996, 104, 2321-2329.	3.0	164
110	Direct Determination of the Quantum-Mechanical Density Matrix Using the Density Equation. Physical Review Letters, 1996, 76, 1039-1042.	7.8	250
111	Electronic mechanism of the surface enhanced Raman scattering. Journal of Chemical Physics, 1995, 103, 2286-2294.	3.0	28
112	Hyperfine splitting constants studied by the symmetry adapted cluster configuration interaction method. Journal of Chemical Physics, 1994, 100, 5821-5828.	3.0	25
113	Spin-spin coupling between the two unpaired electrons in bis(tetrathiafulvalenyl)ketone dications. Advanced Materials, 1993, 5, 741-743.	21.0	25
114	Ferromagnetic Interaction in Organic Radical Ion Salts. Molecular Crystals and Liquid Crystals, 1993, 232, 117-134.	0.3	10
115	Exponentially generated configuration interaction (EGCI) method applied to high spin multiplicity. Journal of Chemical Physics, 1993, 99, 1952-1961.	3.0	11
116	Symmetry adapted cluster configuration interaction method applied to high spin multiplicity. Journal of Chemical Physics, 1993, 98, 7179-7184.	3.0	43
117	Dipped adcluster model study for molecular and dissociative chemisorptions of O ₂ on Ag surface. Journal of Chemical Physics, 1993, 98, 2423-2436.	3.0	75
118	Electronic Theory of the Chemisorption and Catalytic Reactions on Metal Surface.. Hyomen Kagaku, 1993, 14, 603-609.	0.0	1
119	Magnetic Properties in Charge-Transfer Complexes of High-Symmetry Organic Acceptors. Materials Research Society Symposia Proceedings, 1992, 247, 417.	0.1	6
120	Theoretical model studies for surface-molecule interacting systems. International Journal of Quantum Chemistry, 1992, 44, 725-736.	2.0	14
121	Exponentially generated configuration interaction theory. Descriptions of excited, ionized, and electron attached states. Journal of Chemical Physics, 1991, 94, 6716-6727.	3.0	65
122	Description of two- and many-electron processes by the SAC-CI method. Chemical Physics Letters, 1991, 177, 331-337.	2.6	181
123	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface: Image force correction and applications to Pd-O ₂ adclusters. Journal of Chemical Physics, 1991, 95, 640-647.	3.0	43
124	Theoretical study on the ground and excited states of MnO ₄ . Journal of Chemical Physics, 1991, 95, 8287-8291.	3.0	58
125	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.	3.0	18
126	Theoretical study for the excited states of MoO ₄ ⁿ⁻ S ₂ ⁿ⁻ (n=0, 1/4) and MoSe ₂ . Journal of Chemical Physics, 1990, 93, 1865-1875.	3.0	23

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127	Potential energy curves of the ground, excited, and ionized states of Ar ₂ studied by the symmetry adapted cluster configuration interaction theory. <i>Journal of Chemical Physics</i> , 1990, 92, 6084-6092.	3.0	28
128	Calculation of isotropic hyperfine coupling constants by the symmetry adapted cluster expansion configuration interaction theory. <i>Journal of Chemical Physics</i> , 1988, 89, 4185-4192.	3.0	35
129	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface. <i>Journal of Chemical Physics</i> , 1987, 87, 4995-5001.	3.0	67
130	Exponentially generated wave functions. <i>Journal of Chemical Physics</i> , 1985, 83, 5743-5748.	3.0	64
131	Multireference cluster expansion theory: MR SAC theory. <i>Journal of Chemical Physics</i> , 1985, 83, 713-722.	3.0	73
132	Cluster expansion of the wave function. Valence and Rydberg excitations and ionizations of ethylene. <i>Journal of Chemical Physics</i> , 1984, 80, 3703-3709.	3.0	71
133	Cluster expansion of the wavefunction, valence and rydberg excitations, ionizations, and inner-valence ionizations of CO ₂ and N ₂ O studied by the sac and sac CI theories. <i>Chemical Physics</i> , 1983, 75, 425-441.	1.9	269
134	Cluster expansion of the wave function. Ionization and excitation spectra of no radical studied by the SAC and SAC-CI theory. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 241-255.	2.0	5
135	Force in SCF theories. Second derivative of potential energy. <i>Journal of Chemical Physics</i> , 1982, 77, 1961-1968.	3.0	20
136	Cluster expansion of the wave function. Electron correlations in singlet and triplet excited states, ionized states, and electron attached states by SAC and SAC-CI theories. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 1301-1313.	2.0	71
137	Cluster expansion of the wavefunction. Electron correlations in ground and excited states by SAC (symmetry-adapted-cluster) and SAC CI theories. <i>Chemical Physics Letters</i> , 1979, 67, 329-333.	2.6	563
138	Cluster expansion of the wavefunction. Calculation of electron correlations in ground and excited states by SAC and SAC CI theories. <i>Chemical Physics Letters</i> , 1979, 67, 334-342.	2.6	323
139	Hidden potentials in classical theorems. <i>Journal of Chemical Physics</i> , 1977, 67, 1312-1318.	3.0	5
140	The Hellmann-Feynman theorem applied to long-range forces. <i>Theoretica Chimica Acta</i> , 1976, 41, 119-131.	0.8	12
141	Equation for the direct determination of the density matrix. <i>Physical Review A</i> , 1976, 14, 41-50.	2.5	235
142	Electrostatic force theory for a molecule and interacting molecules. I. Concept and illustrative applications. <i>Journal of the American Chemical Society</i> , 1973, 95, 345-354.	13.7	100
143	On the orbital theories in the spin correlation problems. II. Unrestricted and spin extended Hartree-Fock theories. <i>Journal of Chemical Physics</i> , 1973, 59, 2586-2595.	3.0	36
144	On the Unrestricted Hartree-Fock Wavefunction. <i>Journal of Chemical Physics</i> , 1969, 51, 3175-3180.	3.0	58