Hiroshi Nakatsuji

List of Publications by Year
in descending order

144	7,020	50170 46	62479 80
papers	citations	h-index	g-index

144	144	144	3119
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	1.2	563
2	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.	1.2	323
3	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.	0.9	269
4	Direct Determination of the Quantum-Mechanical Density Matrix Using the Density Equation. Physical Review Letters, 1996, 76, 1039-1042.	2.9	250
5	Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm. Journal of Chemical Physics, 2001, 114, 8282-8292.	1.2	239
6	Equation for the direct determination of the density matrix. Physical Review A, 1976, 14, 41-50.	1.0	235
7	Description of two- and many-electron processes by the SAC-CI method. Chemical Physics Letters, 1991, 177, 331-337.	1.2	181
8	Excited and ionized states of free base porphin studied by the symmetry adapted clusterâ€configuration interaction (SACâ€CI) method. Journal of Chemical Physics, 1996, 104, 2321-2329.	1.2	164
9	Solving the SchrÃ¶dinger equation for helium atom and its isoelectronic ions with the free iterative complement interaction (ICI) method. Journal of Chemical Physics, 2007, 127, 224104.	1.2	142
10	Theoretical Studies on the Color-Tuning Mechanism in Retinal Proteins. Journal of Chemical Theory and Computation, 2007, 3, 605-618.	2.3	134
11	Red Light in Chemiluminescence and Yellow-Green Light in Bioluminescence:Â Color-Tuning Mechanism of Firefly,Photinus pyralis, Studied by the Symmetry-Adapted Clusterâ^'Configuration Interaction Method. Journal of the American Chemical Society, 2007, 129, 8756-8765.	6.6	127
12	Structure of the exact wave function. Journal of Chemical Physics, 2000, 113, 2949-2956.	1.2	117
13	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.	1.2	108
14	Quasirelativistic theory for magnetic shielding constants. II. Gauge-including atomic orbitals and applications to molecules. Journal of Chemical Physics, 2003, 118, 1027-1035.	1.2	103
15	Electrostatic force theory for a molecule and interacting molecules. I. Concept and illustrative applications. Journal of the American Chemical Society, 1973, 95, 345-354.	6.6	100
16	Scaled SchrÃ¶dinger Equation and the Exact Wave Function. Physical Review Letters, 2004, 93, 030403.	2.9	96
17	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted clusterâ€"configuration interaction method. Journal of Chemical Physics, 2000, 113, 7853-7866.	1.2	88
18	SAC-CI Method: Theoretical Aspects and Some Recent Topics. Computational Chemistry - Reviews of Current Trends, 1997, , 62-124.	0.4	86

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19	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.	1.2	84
20	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-CI study. Journal of Computational Chemistry, 2003, 24, 1421-1431.	1.5	83
21	Ab initio molecular orbital model of scanning tunneling microscopy. Journal of Chemical Physics, 1996, 104, 2410-2417.	1.2	80
22	Density matrix variational theory: Application to the potential energy surfaces and strongly correlated systems. Journal of Chemical Physics, 2002, 116, 5432-5439.	1.2	79
23	Excited states of GFP chromophore and active site studied by the SACâ€CI method: Effect of proteinâ€environment and mutations. Journal of Computational Chemistry, 2007, 28, 2443-2452.	1.5	78
24	Helical Structure and Circular Dichroism Spectra of DNA: A Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 42-55.	1.1	77
25	Dipped adcluster model study for molecular and dissociative chemisorptions of O2 on Ag surface. Journal of Chemical Physics, 1993, 98, 2423-2436.	1.2	75
26	Multireference cluster expansion theory: MRâ€“SAC theory. Journal of Chemical Physics, 1985, 83, 713-722.	1.2	73
27	Excited States of Free Base Phthalocyanine Studied by the SAC-CI Method. Journal of Physical Chemistry A, 1997, 101, 446-451.	1.1	72
28	Cluster expansion of the wave function. Electron correlations in singlet and triplet excited states, ionized states, and electron attached states bySAC andSAC-CI theories. International Journal of Quantum Chemistry, 1981, 20, 1301-1313.	1.0	71
29	Cluster expansion of the wave function. Valence and Rydberg excitations and ionizations of ethylene. Journal of Chemical Physics, 1984, 80, 3703-3709.	1.2	71
30	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface. Journal of Chemical Physics, 1987, 87, 4995-5001.	1.2	67
31	Mechanism of color tuning in retinal protein: SAC-CI and QM/MM study. Chemical Physics Letters, 2005, 414, 239-242.	1.2	67
32	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.	1.2	66
33	Exponentially generated configuration interaction theory. Descriptions of excited, ionized, and electron attached states. Journal of Chemical Physics, 1991, 94, 6716-6727.	1.2	65
34	Exponentially generated wave functions. Journal of Chemical Physics, 1985, 83, 5743-5748.	1.2	64
35	Structure of the exact wave function. II. Iterative configuration interaction method. Journal of Chemical Physics, 2001, 115, 2000-2006.	1.2	59
36	On the Unrestricted Hartreeâ€“Fock Wavefunction. Journal of Chemical Physics, 1969, 51, 3175-3180.	1.2	58

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37	Theoretical study on the ground and excited states of MnOâ¯4. Journal of Chemical Physics, 1991, 95, 8287-8291.	1.2	58
38	Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SACâ€“CI (configuration interaction) method. Chemical Physics, 1999, 242, 177-193.	0.9	57
39	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.	1.0	55
40	Analytically Solving the Relativistic Dirac-Coulomb Equation for Atoms and Molecules. Physical Review Letters, 2005, 95, 050407.	2.9	54
41	Discovery of a General Method of Solving the SchrÃ¶dinger and Dirac Equations That Opens a Way to Accurately Predictive Quantum Chemistry. Accounts of Chemical Research, 2012, 45, 1480-1490.	7.6	53
42	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. Journal of Chemical Physics, 2002, 117, 2045-2052.	1.2	52
43	Deepening and Extending the Quantum Principles in Chemistry. Bulletin of the Chemical Society of Japan, 2005, 78, 1705-1724.	2.0	51
44	General method of solving the SchrÃ¶dinger equation of atoms and molecules. Physical Review A, 2005, 72, .	1.0	51
45	A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. Organometallics, 2008, 27, 1736-1742.	1.1	47
46	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.	1.2	46
47	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.	1.2	46
48	Free iterative-complement-interaction calculations of the hydrogen molecule. Physical Review A, 2005, 72, .	1.0	45
49	Solving non-Bornâ€“Oppenheimer SchrÃ¶dinger equation for hydrogen molecular ion and its isotopomers using the free complement method. Journal of Chemical Physics, 2009, 130, 024102.	1.2	45
50	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface: Image force correction and applications to Pdâ€“O2 adclusters. Journal of Chemical Physics, 1991, 95, 640-647.	1.2	43
51	Symmetryâ€adapted clusterâ€“configuration interaction method applied to highâ€spin multiplicity. Journal of Chemical Physics, 1993, 98, 7179-7184.	1.2	43
52	Structure of the exact wave function. III. Exponential ansatz. Journal of Chemical Physics, 2001, 115, 2465-2475.	1.2	43
53	Solving the SchrÃ¶dinger 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.	1.3	42
54	Artificial color tuning of firefly luminescence: Theoretical mutation by tuning electrostatic interactions between protein and luciferin. Chemical Physics Letters, 2009, 469, 191-194.	1.2	39

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55	Inverse SchrÃ¶dinger equation and the exact wave function. Physical Review A, 2002, 65, .	1.0	38
56	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.	1.2	37
57	Ionized and excited states of ferrocene: Symmetry adapted clusterâ€"configurationâ€"interaction study. Journal of Chemical Physics, 2002, 117, 6533-6537.	1.2	37
58	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.	1.2	37
59	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.	1.2	37
60	On the orbital theories in the spinâ€correlation problems. II. Unrestricted and spinâ€extended Hartreeâ€Fock theories. Journal of Chemical Physics, 1973, 59, 2586-2595.	1.2	36
61	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.	1.5	36
62	On the color-tuning mechanism of Human-Blue visual pigment: SAC-CI and QM/MM study. Chemical Physics Letters, 2006, 432, 252-256.	1.2	36
63	Calculation of isotropic hyperfine coupling constants by the symmetry adapted cluster expansion configuration interaction theory. Journal of Chemical Physics, 1988, 89, 4185-4192.	1.2	35
64	Self-Condensation Reaction of Lithium (Alkoxy)silylenoid:Â A Model Study by ab Initio Calculation. Organometallics, 1998, 17, 4573-4577.	1.1	35
65	How Accurately Does the Free Complement Wave Function of a Helium Atom Satisfy the SchrÃ¶dinger Equation?. Physical Review Letters, 2008, 101, 240406.	2.9	35
66	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.	2.0	35
67	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.	1.2	34
68	Symmetry-adapted-cluster/symmetry-adapted-cluster configuration interaction methodology extended to giant molecular systems: Ring molecular crystals. Journal of Chemical Physics, 2007, 126, 084104.	1.2	34
69	SAC-CI GENERAL-R METHOD: THEORY AND APPLICATIONS TO THE MULTI-ELECTRON PROCESSES. , 2002, , 293-319.		33
70	Peralkylated Tetrasilanes:Â Conformational Dependence of the Photoelectron Spectrumâ€. Journal of Physical Chemistry A, 2002, 106, 2369-2373.	1.1	33
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.	1.2	32
72	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.	1.2	32

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73	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. Journal of Chemical Physics, 2002, 116, 1811-1824.	1.2	31
74	LiH potential energy curves for ground and excited states with the free complement local SchrÃ¶dinger equation method. Chemical Physics Letters, 2010, 496, 347-350.	1.2	29
75	Potential energy curves of the ground, excited, and ionized states of Ar2 studied by the symmetry adapted clusterâ€configuration interaction theory. Journal of Chemical Physics, 1990, 92, 6084-6092.	1.2	28
76	Electronic mechanism of the surface enhanced Raman scattering. Journal of Chemical Physics, 1995, 103, 2286-2294.	1.2	28
77	Solving the SchrÃ¶dinger and Dirac equations of hydrogen molecular ion accurately by the free iterative complement interaction method. Journal of Chemical Physics, 2008, 128, 124103.	1.2	28
78	Accurate solutions of the SchrÃ¶dinger and Dirac equations of , HD+, and HT+: With and without Bornâ€“Oppenheimer approximation and under magnetic field. Chemical Physics, 2012, 401, 62-72.	0.9	26
79	Similarities and Differences between RNA and DNA Double-Helical Structures in Circular Dichroism Spectroscopy: A SACâ€“CI Study. Journal of Physical Chemistry A, 2016, 120, 9008-9018.	1.1	26
80	Spin-spin coupling between the two unpaired electrons in bis(tetrathiafulvalenyl)ketone dications. Advanced Materials, 1993, 5, 741-743.	11.1	25
81	Hyperfine splitting constants studied by the symmetry adapted clusterâ€configuration interaction method. Journal of Chemical Physics, 1994, 100, 5821-5828.	1.2	25
82	Quasirelativistic study of125Te nuclear magnetic shielding constants and chemical shifts. Journal of Computational Chemistry, 2001, 22, 1502-1508.	1.5	25
83	Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. International Journal of Quantum Chemistry, 1997, 65, 839-855.	1.0	24
84	Theoretical study for the excited states of MoO4â^'nS2â^'n(n=0â^¼4) and MoSe2â^'4. Journal of Chemical Physics, 1990, 93, 1865-1875.	1.2	23
85	Force in SCF theories. Second derivative of potential energy. Journal of Chemical Physics, 1982, 77, 1961-1968.	1.2	20
86	Outer- and inner-valence ionization spectra of NH3, PH3, and AsH3: symmetry-adapted cluster configuration interaction general-R study. Journal of Chemical Physics, 2002, 116, 1934-1943.	1.2	20
87	Free-complement local-SchrÃ¶dinger-equation method for solving the SchrÃ¶dinger equation of atoms and molecules: Basic theories and features. Journal of Chemical Physics, 2015, 142, 084117.	1.2	20
88	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis:â€‰ Theoretical Study. Journal of Physical Chemistry B, 2003, 107, 838-847.	1.2	19
89	SAC and SACâ^'CI Calculations of Excitation and Circular Dichroism Spectra of Straight-Chain and Cyclic Dichalcogens. Journal of Physical Chemistry A, 2006, 110, 10053-10062.	1.1	19
90	SOLVING THE SCHRÃ–DINGER AND DIRAC EQUATIONS FOR A HYDROGEN ATOM IN THE UNIVERSE'S STRONGEST MAGNETIC FIELDS WITH THE FREE COMPLEMENT METHOD. Astrophysical Journal, 2010, 725, 528-533.	1.6	19

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91	Mixedâ€exponentially generated wave function method for ground, excited, ionized, and electron attached states of a molecule. Journal of Chemical Physics, 1991, 95, 4296-4305.	1.2	18
92	Roles of proteins in the electron transfer in the photosynthetic reaction center ofRhodopseudomonas viridis: bacteriopheophytin to ubiquinone. Journal of Computational Chemistry, 2001, 22, 265-272.	1.5	16
93	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.	1.2	16
94	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.	2.0	16
95	Solving the SchrÃ¶dinger equation of atoms and molecules: Chemical-formula theory, free-complement chemical-formula theory, and intermediate variational theory. Journal of Chemical Physics, 2018, 149, 114105.	1.2	16
96	CASSCF study of bonding in NiCO and FeCO. International Journal of Quantum Chemistry, 1999, 72, 221-231.	1.0	15
97	General coalescence conditions for the exact wave functions: Higher-order relations for two-particle systems. Journal of Chemical Physics, 2013, 139, 044114.	1.2	15
98	Non-Born-Oppenheimer potential energy curve: Hydrogen molecular ion with highly accurate free complement method. Journal of Chemical Physics, 2013, 139, 074105.	1.2	15
99	SOLVING THE NON-BORN-OPPENHEIMER SCHRÃ–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.	1.6	15
100	Indicator of the Stacking Interaction in the DNA Double-Helical Structure: ChiraSac Study. Journal of Physical Chemistry A, 2015, 119, 8269-8278.	1.1	15
101	Solving the SchrÃ¶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.	1.2	15
102	Theoretical model studies for surface-molecule interacting systems. International Journal of Quantum Chemistry, 1992, 44, 725-736.	1.0	14
103	Conformational Dependence of the Circular Dichroism Spectrum of Î±-Hydroxyphenylacetic Acid: A ChiraSac Study. Journal of Physical Chemistry A, 2013, 117, 14065-14074.	1.1	14
104	Circular Dichroism Spectra of Uridine Derivatives: ChiraSac Study. Journal of Physical Chemistry A, 2014, 118, 2931-2941.	1.1	14
105	Analytical evaluations of exponentially correlated unlinked one-center, three- and four-electron integrals. Physical Review A, 2012, 85, .	1.0	13
106	Solving the SchrÃ¶dinger 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 Î£ symmetry. Physical Chemistry Chemical Physics, 2019, 21, 6327-6340.	1.3	13
107	The Hellmann-Feynman theorem applied to long-range forces. Theoretica Chimica Acta, 1976, 41, 119-131.	0.9	12
108	Equation for the direct determination of the density matrix: Time-dependent density equation and perturbation theory. Theoretical Chemistry Accounts, 1999, 102, 97-104.	0.5	12

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109	Electronic circular dichroism spectrum of uridine studied by the SACâ€“CI method. Chemical Physics Letters, 2006, 425, 367-371.	1.2	12
110	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.	1.0	12
111	Electronic excitation spectra of doublet anion radicals of cyanobenzene and nitrobenzene derivatives: SAC-CI theoretical studies. Molecular Physics, 2015, 113, 1728-1739.	0.8	12
112	Solving the SchrÃ¶dinger equation of molecules by relaxing the antisymmetry rule: Inter-exchange theory. Journal of Chemical Physics, 2015, 142, 194101.	1.2	12
113	Exponentially generated configuration interaction (EGCI) method applied to highâ€spin multiplicity. Journal of Chemical Physics, 1993, 99, 1952-1961.	1.2	11
114	Ferromagnetic Interaction in Organic Radical Ion Salts. Molecular Crystals and Liquid Crystals, 1993, 232, 117-134.	0.3	10
115	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.	1.2	10
116	Solving the SchrÃ¶dinger 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.	1.2	10
117	Solving the SchrÃ¶dinger equation of atoms and molecules using one- and two-electron integrals only. Physical Review A, 2020, 101, .	1.0	10
118	Exploring Photobiology and Biospectroscopy with the Sac-Ci (Symmetry-Adapted) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (Cluster- and Physics, 2008, , 93-124.	0.6	9
119	Accuracy of Td-DFT in the Ultraviolet and Circular Dichroism Spectra of Deoxyguanosine and Uridine. Journal of Physical Chemistry A, 2018, 122, 100-118.	1.1	9
120	Electron transfer in the c-type cytochrome subunit of the photosynthetic reaction center ofRhodopseudomonas viridis:ab initio theoretical study. Journal of Computational Chemistry, 2001, 22, 521-527.	1.5	8
121	Solving the SchrÃ¶dinger equation of hydrogen molecule with the free complementâ€“local SchrÃ¶dinger equation method: Potential energy curves of the ground and singly excited singlet and triplet states, Î£, Î, Î”, and Î¦. Journal of Chemical Physics, 2018, 149, 244116.	1.2	8
122	Light-Driven Proton, Sodium Ion, and Chloride Ion Transfer Mechanisms in Rhodopsins: SAC-CI Study. Journal of Physical Chemistry A, 2019, 123, 1766-1784.	1.1	8
123	Efficient antisymmetrization algorithm for the partially correlated wave functions in the free complement-local SchrÃ¶dinger equation method. Journal of Chemical Physics, 2013, 139, 044112.	1.2	7
124	Magnetic Properties in Charge-Transfer Complexes of High-Symmetry Organic Acceptors. Materials Research Society Symposia Proceedings, 1992, 247, 417.	0.1	6
125	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.	1.3	6
126	Accurate scaling functions of the scaled SchrÃ¶dinger equation. Journal of Chemical Physics, 2022, 156, 014113.	1.2	6

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127	Hidden potentials in classical theorems. Journal of Chemical Physics, 1977, 67, 1312-1318.	1.2	5
128	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, 239-247.	2.3	5
129	Valence ionization spectra of 4Ï€-electron molecules with low-lying satellites involving nâ€“Ï€* and Ï€â€“Ï€* transitions. Molecular Physics, 2006, 104, 971-982.	0.8	5
130	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, 1983, 24, 241-255.	1.0	5
131	Free complement <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>s</mml:mi><mml:mrow><mml:mi>i</mml:mi><mml:mi>j</mml:mi></mml:mrow></mml:msub></mml:math>-assisted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>r</mml:mi><mml:mrow><mml:mi>i</mml:mi><mml:mi>j</mml:mi></mml:mrow></mml:msub></mml:math> theory: Variational calculation of the quintet state of a carbon atom. Physical Review A, 2020, 102, .	1.0	5
132	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.	0.8	4
133	Theoretical Study on the Thermal and Photochemical Isomerization Reactions of Dicyanoacetylene Complex of Platinum Pt(PH3)2(C4N2). Journal of Physical Chemistry A, 1997, 101, 973-980.	1.1	3
134	Solving the SchrÃ¶dinger 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 Î symmetry. Physical Chemistry Chemical Physics, 2020, 22, 13489-13497.	1.3	3
135	Circular Dichroism Spectroscopy with the SAC-CI Methodology: A ChiraSac Study. , 2018, , 21-47.		1
136	Photoelectron spectrum of NO2â¯: SACâ€CI gradient study of vibrationalâ€rotational structures. Journal of Computational Chemistry, 2019, 40, 360-374.	1.5	1
137	CASSCF study of bonding in NiCO and FeCO. , 1999, 72, 221.		1
138	Electronic Theory of the Chemisorption and Catalytic Reactions on Metal Surface.. Hyomen Kagaku, 1993, 14, 603-609.	0.0	1
139	GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMILTONIANS. Recent Advances in Computational, 2004, , 191-220.	0.8	0
140	Photochemistry of Organic Light-Emitting Diodes. AIP Conference Proceedings, 2007, , .	0.3	0
141	Photochemistry of Biological Chemosensors, Organic Light-Emitting Diodes, and Inner-shell Electronic Processes. AIP Conference Proceedings, 2008, , .	0.3	0
142	Electronic structure and optical properties of conjugated molecules: SAC-CI study. , 2012, , .		0
143	Keiji Morokuma. Journal of Physical Chemistry A, 2018, 122, 880-881.	1.1	0
144	STRUCTURE OF THE EXACT WAVE FUNCTION: PROGRESS REPORT. , 2003, , .		0