

# Suehiro Iwata

## List of Publications by Year in descending order

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g-index

150  
all docs

150  
docs citations

150  
times ranked

2471  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic spectra of ion radicals and their molecular orbital interpretation. III. Aromatic hydrocarbons. Journal of the American Chemical Society, 1973, 95, 3473-3483.	13.7	323
2	Molecular Orbital Studies of the Structures and Reactions of Singly Charged Magnesium Ion with Water Clusters, Mg+(H <sub>2</sub> O) <sub>n</sub> . Journal of the American Chemical Society, 1995, 117, 755-763.	13.7	130
3	Photodissociation of size-selected aquamagnesium (Mg+(H <sub>2</sub> O) <sub>n</sub> ) ions for n = 1 and 2. The Journal of Physical Chemistry, 1992, 96, 8259-8264.	2.9	126
4	Molecular Complexes between 1,2,4,5-Tetracyanobenzene and Some Aromatic Electron Donors. Journal of the American Chemical Society, 1966, 88, 894-902.	13.7	123
5	Phosphorescence of the Charge-Transfer Triplet States of Some Molecular Complexes. Journal of Chemical Physics, 1967, 47, 2203-2209.	3.0	122
6	Theoretical studies of geometric structures of phenol-water clusters and their infrared absorption spectra in the O-H stretching region. Journal of Chemical Physics, 1996, 105, 420-431.	3.0	110
7	The geometric and electronic structures of Ar <sub>n</sub> <sup>+</sup> (n=3-27). Journal of Chemical Physics, 1993, 98, 3038-3048.	3.0	107
8	Ab initio evaluation of correlation contributions to the true electron Hamiltonian: Ethylene. Journal of Chemical Physics, 1974, 61, 1500-1509.	3.0	93
9	Photoelectron spectroscopy of silicon-carbon cluster anions (SiC <sub>n</sub> <sup>-m</sup> ). Journal of Chemical Physics, 1995, 103, 2050-2057.	3.0	82
10	An MCSCF study of the low-lying states of trans-butadiene. Journal of Chemical Physics, 1985, 83, 1140-1148.	3.0	81
11	Geometric and electronic structures of silicon-sodium binary clusters. I. Ionization energy of Si <sub>n</sub> Na <sub>m</sub> . Journal of Chemical Physics, 1997, 107, 3056-3070.	3.0	80
12	Basis set superposition error free self-consistent field method for molecular interaction in multi-component systems: Projection operator formalism. Journal of Chemical Physics, 2001, 115, 3553-3560.	3.0	75
13	ESR Spectra of the Charge-Transfer Triplet States of Some Molecular Complexes. Journal of Chemical Physics, 1969, 50, 993-1000.	3.0	73
14	Ab Initio Studies of Aromatic Excimers Using Multiconfiguration Quasi-Degenerate Perturbation Theory. Journal of Physical Chemistry A, 2011, 115, 7687-7699.	2.5	73
15	Molecular orbital studies of hydrogen bonds. V. Analysis of the hydrogen-bond energy between lower excited states of formaldehyde and water. Journal of the American Chemical Society, 1973, 95, 7563-7575.	13.7	71
16	Absorption and emission spectra of 1,2,4,5-tetracyanobenzene-naphthalene complex crystal. Journal of the American Chemical Society, 1967, 89, 2813-2819.	13.7	67
17	Resonance Raman and FTIR Spectra of Isotope-Labeled Reduced 1,4-Benzoquinone and Its Protonated Forms in Solutions. Journal of Physical Chemistry A, 1997, 101, 622-631.	2.5	67
18	Density functional crystal orbital study on the normal vibrations of polyacetylene and polymethineimine. Journal of Chemical Physics, 1997, 107, 10075-10084.	3.0	66

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19	Absorption Spectra of Dianthracene Anion Radical and Anthracene Dimer Anion. Journal of Chemical Physics, 1972, 56, 2858-2864.	3.0	65
20	Nonclassical terms in the true effective valence shell Hamiltonian: A second quantized formalism. Journal of Chemical Physics, 1976, 65, 1071-1088.	3.0	63
21	Photodissociation of Ar <sup>+</sup> 3 cluster ion. Chemical Physics Letters, 1990, 171, 433-438.	2.6	62
22	Theoretical Studies of Structures and Ionization Threshold Energies of Water Cluster Complexes with a Group 1 Metal, M(H <sub>2</sub> O) <sub>n</sub> (M = Li and Na). Journal of Physical Chemistry A, 1999, 103, 6134-6141.	2.5	61
23	Electronic spectra and electronic structures of [2.2]paracyclophane and related compounds. Journal of Molecular Spectroscopy, 1973, 46, 1-15.	1.2	60
24	Promotion of the proton transfer reaction by the intermolecular stretching mode: Application of the two-dimensional finite element method to the nuclear Schrödinger equation. Journal of Chemical Physics, 1988, 89, 2932-2937.	3.0	59
25	Photoelectron spectroscopy of silicon-fluorine binary cluster anions (SiF <sub>n</sub> <sup>-m</sup> ). Journal of Chemical Physics, 1996, 105, 5369-5376.	3.0	58
26	Electronic absorption spectra of excess electrons in molecular aggregates. I. Trapped electrons in $\gamma$ -irradiated amorphous solids at 77.deg.K. The Journal of Physical Chemistry, 1972, 76, 3683-3691.	2.9	56
27	Geometric and electronic structures of silicon-sodium binary clusters. II. Photoelectron spectroscopy of Si <sub>n</sub> Na <sup>m-</sup> cluster anions. Journal of Chemical Physics, 1997, 107, 10029-10043.	3.0	56
28	Ab Initio Studies on the Structures, Vertical Electron Detachment Energies, and Fragmentation Energies of C <sub>n</sub> B-Clusters. Journal of Physical Chemistry A, 1997, 101, 591-596.	2.5	53
29	Dipole-bound and interior electrons in water dimer and trimer anions: ab initio MO studies. Chemical Physics Letters, 1998, 287, 553-562.	2.6	52
30	Electron-hydrogen bonds and OH harmonic frequency shifts in water cluster complexes with a group 1 metal atom, M(H <sub>2</sub> O) <sub>n</sub> (M=Li and Na). Journal of Chemical Physics, 2000, 112, 5705-5710.	3.0	52
31	Potential energy curves of several excited states of the Ne <sub>2</sub> <sup>*</sup> excimer: Assignment of the transient absorption spectra of the excimer. Chemical Physics, 1979, 37, 251-257.	1.9	51
32	Accurate potential energy and transition dipole moment curves for several electronic states of CO <sup>+</sup> . Journal of Chemical Physics, 2000, 112, 1804-1808.	3.0	49
33	Ab initio MO studies of neutral and anionic SiC <sub>n</sub> clusters (n=2-5). Journal of Chemical Physics, 1997, 107, 10051-10061.	3.0	48
34	Analytical energy gradients in second-order Møller-Plesset perturbation theory for extended systems. Journal of Chemical Physics, 1998, 109, 4147-4155.	3.0	48
35	Breakdown of Koopmans' theorem and strong shake-up bands in the valence shell region of N <sub>2</sub> photoelectron spectra. Chemical Physics, 1979, 39, 337-349.	1.9	45
36	Molecular orbital studies of hydrogen bonds. Theoretica Chimica Acta, 1977, 44, 323-339.	0.8	44

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37	Three-center expansion of electron repulsion integrals with linear combination of atomic electron distributions. <i>Chemical Physics Letters</i> , 1995, 240, 578-584.	2.6	44
38	Theoretical studies of the water-cluster anions containing the OH <sub>e</sub> HO structure: energies and harmonic frequencies. <i>Chemical Physics Letters</i> , 1999, 315, 433-440.	2.6	44
39	Molecular Orbital Studies of the Structures and Reactions of a Singly Charged Calcium Ion with Water Clusters, Ca <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> . <i>Journal of Physical Chemistry A</i> , 1997, 101, 487-496.	2.5	43
40	Theoretical molecular Auger spectra with electron population analysis. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003, 128, 103-117.	1.7	43
41	Theoretical study of multidimensional proton tunneling in the excited state of tropolone. <i>Journal of Chemical Physics</i> , 2000, 112, 6322-6328.	3.0	42
42	Valence type vacant orbitals for configuration interaction calculations. <i>Chemical Physics Letters</i> , 1981, 83, 134-138.	2.6	41
43	Electronic spectra of ion-radicals and their molecular orbital interpretation. I. Aromatic nitro-substituted anion-radicals. <i>The Journal of Physical Chemistry</i> , 1971, 75, 2591-2602.	2.9	40
44	Theoretical study of hydrated Be <sup>2+</sup> ions. <i>Chemical Physics</i> , 1987, 116, 193-202.	1.9	40
45	Structures, Spectroscopies, and Reactions of Atomic Ions with Water Clusters. <i>Advances in Chemical Physics</i> , 2007, , 431-523.	0.3	39
46	Static structure factor and electron correlation effects studied by inelastic x-ray scattering spectroscopy. <i>Journal of Chemical Physics</i> , 1998, 108, 4545-4553.	3.0	38
47	Theoretical Studies of the Aluminum <sup>+</sup> Water Clusters Al(H <sub>2</sub> O) <sub>n</sub> and Their Ions [Al(H <sub>2</sub> O) <sub>n</sub> ] <sup>+</sup> . <i>Bulletin of the Chemical Society of Japan</i> , 1993, 66, 3245-3252.	3.2	37
48	Ab initio studies on the structures and vertical electron detachment energies of copper-water negative ion clusters Cu <sup>-</sup> (H <sub>2</sub> O) <sub>n</sub> and CuOH <sup>-</sup> (H <sub>2</sub> O) <sub>n-1</sub> . <i>Chemical Physics Letters</i> , 1995, 232, 72-78.	2.6	37
49	Theoretical Studies of Boron <sup>+</sup> Water Cluster Ions B <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> and Aluminum <sup>+</sup> Water Cluster Ions Al <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> : Isomers and Intracuster Reactions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 3377-3386.	2.9	37
50	Geometric and electronic structures of fluorine bound silicon clusters. <i>Journal of Chemical Physics</i> , 1998, 108, 8039-8058.	3.0	37
51	Molecular orbital studies of hydrogen bonds. VI. Origin of red shift of .pi.-.pi.* transitions. trans-Acrolein-water complex. <i>Journal of the American Chemical Society</i> , 1975, 97, 966-970.	13.7	36
52	Multiconfiguration self-consistent field procedure employing linear combination of atomic electron distributions. <i>Journal of Chemical Physics</i> , 1996, 105, 3604-3611.	3.0	35
53	Density functional crystal orbital study on the normal vibrations and phonon dispersion curves of all-trans polyethylene. <i>Journal of Chemical Physics</i> , 1998, 108, 7901-7908.	3.0	34
54	Perturbation expansion theory corrected from basis set superposition error. I. Locally projected excited orbitals and single excitations. <i>Journal of Chemical Physics</i> , 2004, 120, 3555-3562.	3.0	34

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55	Double breakdown of Koopmans' theorem and strong correlation satellites in the He II photoelectron spectrum of O <sub>3</sub> . <i>Chemical Physics</i> , 1981, 58, 267-273.	1.9	33
56	Ab Initio Studies of Silicon and Nitrogen Clusters: A Cyclic or Linear Si <sub>2</sub> N <sub>3</sub> ? <i>The Journal of Physical Chemistry</i> , 1996, 100, 10919-10927.	2.9	33
57	Theoretical study of the photoabsorption cross sections of HOCl and HOF. <i>Chemical Physics</i> , 1989, 135, 75-83.	1.9	32
58	Ab initio studies on the structures, vertical electron detachment energies, and stabilities of C <sub>n</sub> P <sup>-</sup> clusters. <i>Journal of Chemical Physics</i> , 1997, 107, 7323-7330.	3.0	32
59	Photoelectron spectroscopy of Al <sub>n</sub> S <sub>1</sub> <sup>-</sup> clusters (n=1~9). <i>Journal of Chemical Physics</i> , 1995, 102, 660-665.	3.0	31
60	Hybrid procedure of ab initio molecular orbital calculation and Monte Carlo simulation for studying intracluster reactions: applications to Mg+(H <sub>2</sub> O) <sub>n</sub> (n = 1~4). <i>Chemical Physics Letters</i> , 1996, 260, 1-6.	2.6	30
61	Molecular orbital studies of hydrogen bonds. IV. Hydrogen bonds in excited states of H <sub>2</sub> CO with H <sub>2</sub> O. <i>Chemical Physics Letters</i> , 1973, 19, 94-98.	2.6	29
62	Ab Initio Hartree-Fock and Density Functional Studies on the Structures and Vibrations of an Infinite Hydrogen Fluoride Polymer. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8426-8436.	2.5	29
63	Electronic Spectra and Structures of Solvated NH <sub>4</sub> Radicals, NH <sub>4</sub> (NH <sub>3</sub> ) <sub>n</sub> (n= 1~8). <i>Journal of Physical Chemistry A</i> , 2002, 106, 5242-5248.	2.5	29
64	Theoretical assignments of the photo-dissociation excitation spectra of Mg <sup>+</sup> ion complexes with water clusters: Multi-reference CI studies. <i>Journal of Chemical Physics</i> , 1998, 108, 10078-10083.	3.0	28
65	Electronic and molecular structure of the water dimer cation. A theoretical study. <i>Chemical Physics Letters</i> , 1983, 95, 579-583.	2.6	27
66	Excitation and dispersed fluorescence spectra of the B <sub>2</sub> (V)-1 <sup>1</sup> g+(X <sub>1</sub> <sup>1</sup> ) transition of jet-cooled CS <sub>2</sub> . <i>Chemical Physics</i> , 1984, 86, 173-188.	1.9	27
67	Theoretical study of carbon doped small silicon clusters: Electron affinities of Si <sub>n</sub> C (n=2~5). <i>Journal of Chemical Physics</i> , 1996, 104, 8593-8604.	3.0	27
68	E.S.R. of the charge-transfer triplet state of the durene-tetracyanobenzene complex. <i>Molecular Physics</i> , 1967, 13, 489-490.	1.7	26
69	The vibrational spectrum of H <sub>2</sub> O <sub>2</sub> +... radical cation: An illustration of symmetry breaking. <i>Journal of Chemical Physics</i> , 1997, 106, 4877-4888.	3.0	26
70	Transannular Interaction in the Excited Triplet States of [2.2]Paracyclophane and Related Compounds. <i>Bulletin of the Chemical Society of Japan</i> , 1979, 52, 1346-1350.	3.2	24
71	Ab initio self-consistent-field molecular orbital study on the hydration of three oxidation states of beryllium in aqueous solution. <i>The Journal of Physical Chemistry</i> , 1989, 93, 2165-2169.	2.9	24
72	Theoretical assignment of the vibronic bands in the photoelectron spectra of N <sub>2</sub> below 30 eV. <i>Chemical Physics Letters</i> , 1993, 211, 319-327.	2.6	24

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73	New time-independent perturbation theory for the multireference problem. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 256-264.	2.0	24
74	Cooperative Roles of Charge Transfer and Dispersion Terms in Hydrogen-Bonded Networks of $(\text{H}_2\text{O})_n$ , $n = 6, 11, \text{ and } 16$ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 6641-6651.	2.5	24
75	Ab initio studies of the $\text{I}^2\text{A}^-$ decay in OHT, NH <sub>2</sub> T, CH <sub>3</sub> T, and 14CH <sub>4</sub> . <i>Journal of Chemical Physics</i> , 1977, 66, 4671-4676.	3.0	23
76	Direct calculation of the frequency-dependent polarizability from a CI matrix. <i>Chemical Physics Letters</i> , 1983, 102, 544-549.	2.6	23
77	Noble Gas Clusters Doped with a Metal Ion I: Ab Initio Studies of Na <sup>+</sup> Ar <sub>n</sub> . <i>Journal of Physical Chemistry A</i> , 2004, 108, 683-690.	2.5	23
78	Fluorescence cross sections and electronic transition moments for the $\text{A}^2\Sigma^+ + \text{X}^2\Sigma^+$ transition in HCl <sup>+</sup> by photoionization. Comparison with the ab initio calculations. <i>Journal of Chemical Physics</i> , 1983, 79, 4805-4810.	3.0	22
79	Application of finite-element method to the two-dimensional Schrödinger equation. <i>Journal of Computational Chemistry</i> , 1988, 9, 222-231.	3.3	22
80	Size dependence of the photoabsorption spectra of Ar <sub>n</sub> , $n=4-25$ : A solvation effect on the Ar <sub>3</sub> chromophore. <i>Journal of Chemical Physics</i> , 1996, 105, 10734-10742.	3.0	22
81	Multi-configuration electron-hole potential method for excited states. <i>Theoretica Chimica Acta</i> , 1974, 33, 285-297.	0.8	21
82	Structures and Energetics of New Nitrogen and Silicon Molecules: An Ab Initio Study of Si <sub>2</sub> N <sub>2</sub> . <i>The Journal of Physical Chemistry</i> , 1996, 100, 16155-16161.	2.9	21
83	Diazasilene (Si <sub>2</sub> N <sub>2</sub> ): Is there a conflict between experiment and theory?. <i>Journal of Chemical Physics</i> , 1997, 106, 151-157.	3.0	21
84	Analysis of hydrogen bond energies and hydrogen bonded networks in water clusters $(\text{H}_2\text{O})_{20}$ and $(\text{H}_2\text{O})_{25}$ using the charge-transfer and dispersion terms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11310-11317.	2.8	21
85	Potential energy curves of low-lying states of HNO. <i>Chemical Physics Letters</i> , 1979, 66, 523-526.	2.6	20
86	Theoretical study of silicon-sodium binary clusters. Geometrical and electronic structures of Si Na (n). <i>Journal of Physical Chemistry</i> , 1996, 100, 16155-16161.	2.6	20
87	Analytical second derivatives in ab initio Hartree-Fock crystal orbital theory of polymers. <i>Computational and Theoretical Chemistry</i> , 1998, 451, 121-134.	1.5	20
88	Size-extensive calculations of static structure factors from the coupled cluster singles and doubles model. <i>Journal of Chemical Physics</i> , 1999, 111, 827-832.	3.0	20
89	Perturbation expansion theory corrected from basis set superposition error II. Charge transfer, pair correlation and dispersion terms. <i>Theoretical Chemistry Accounts</i> , 2006, 117, 137-144.	1.4	20
90	Analysis of the oxidation state and oxidation number by ab initio molecular orbital calculations: chlorine and sulfur compounds. <i>Journal of the American Chemical Society</i> , 1982, 104, 3998-4005.	13.7	19

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91	Ab initio study of structure and stability of beryllium compounds. Computational and Theoretical Chemistry, 1987, 152, 101-117.	1.5	18
92	Theoretical Study on the Weakly-Bound Complexes in the Reactions of Hydroxyl Radical with Saturated Hydrocarbons (Methane, Ethane, and Propane). Journal of Physical Chemistry A, 2002, 106, 2652-2658.	2.5	18
93	Analysis of exact valence shell hamiltonian: Nonclassical terms and molecular based parameters. Chemical Physics Letters, 1976, 38, 425-431.	2.6	17
94	Ab initio studies on the vacuum ultraviolet (VUV) excimer emission spectra of NeB <sup>+</sup> and ArB <sup>+</sup> . Journal of Chemical Physics, 1985, 82, 2346-2351.	3.0	17
95	Ab Initio Study of Photochemical Reactions of Ammonia Dimer Systems. Journal of Physical Chemistry A, 1997, 101, 3613-3618.	2.5	17
96	Molecular Interactions in Ground and Excited States. , 1974, , 277-316.		17
97	Solution of large configuration mixing matrices arising in partitioning technique and applications to the generalized eigenvalue problem. Chemical Physics, 1975, 11, 433-440.	1.9	16
98	Molecular orbital study on the mechanism of oxidation of a beryllium atom in acidic solution. Journal of the American Chemical Society, 1990, 112, 7189-7196.	13.7	16
99	Assignment of the photoelectron spectrum of HCl above 20 eV. Chemical Physics Letters, 1993, 210, 187-192.	2.6	16
100	Application of the higher order finite-element method to one-dimensional Schrödinger equation. Journal of Computational Chemistry, 1988, 9, 827-835.	3.3	15
101	Ab Initio Molecular Orbital Study on the Excited States of [2.2]-, [3.3]-, and Siloxane-Bridged Paracyclophanes. Journal of Physical Chemistry A, 2012, 116, 10194-10202.	2.5	15
102	Theoretical Studies of Ammonia-Halogen and Methylamine-Halogen Complexes: Geometries, Harmonic Vibrational Frequencies and Their Infrared Intensities, and Excited States of Ammonia-Chlorine Monofluoride Complex. Bulletin of the Chemical Society of Japan, 1994, 67, 3172-3178.	3.2	14
103	Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion. Chemical Physics, 1998, 230, 45-56.	1.9	14
104	Dispersion energy evaluated by using locally projected occupied and excited molecular orbitals for molecular interaction. Journal of Chemical Physics, 2011, 135, 094101.	3.0	14
105	Electronic absorption spectra of excess electrons in molecular aggregates. II. Solvated electrons. The Journal of Physical Chemistry, 1972, 76, 3691-3694.	2.9	13
106	Quantum chemical interpretation of oxidation number as applied to carbon and oxygen compounds. Numerical analysis of the electron distribution with ab initio molecular orbital wave functions. Journal of the American Chemical Society, 1984, 106, 2787-2792.	13.7	13
107	Ab Initio Studies of the Hydrogen Atom Addition to Ethylene. Bulletin of the Chemical Society of Japan, 1980, 53, 61-67.	3.2	12
108	Theoretical studies of vacuum ultraviolet emission spectra of NeLi <sup>+</sup> and ArLi <sup>+</sup> . Journal of Chemical Physics, 1991, 94, 3707-3714.	3.0	12

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109	<i>Ab initio</i> Monte Carlo simulation using multicanonical algorithm: temperature dependence of the average structure of water dimer. <i>Molecular Physics</i> , 1999, 96, 349-358.	1.7	12
110	Theoretical studies on the molecular dependence of the bond dissociation after the core excitations. CH <sub>3</sub> OCO(CH <sub>2</sub> ) <sub>n</sub> CN, n=0, 1, 2. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2001, 120, 137-148.	1.7	12
111	Theabinitipotential energy surfaces of some low-lying states of acetylene. <i>Journal of Chemical Physics</i> , 1981, 74, 6830-6841.	3.0	11
112	Ab initio studies of the low-lying states of BeO. <i>Theoretica Chimica Acta</i> , 1992, 81, 223-235.	0.8	11
113	Theoretical study of vibrational spectra for Cl <sup>+</sup> (H <sub>2</sub> O): temperature dependence and the influence of Ar (n=1-3). <i>Chemical Physics Letters</i> , 1999, 312, 522-529.	2.6	11
114	Ab initio MO study of the A, D and third 2 <sup>1</sup> states of CO <sup>+</sup> . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2000, 108, 225-234.	1.7	11
115	Energy analysis of weak electron-donor-acceptor complexes and water clusters with the perturbation theory based on the locally projected molecular orbitals: charge-transfer and dispersion terms. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7787.	2.8	11
116	Charge-Transfer Complexes of Maleic Anhydride and Dichloromaleic Anhydride with Various Aromatic Compounds. <i>Bulletin of the Chemical Society of Japan</i> , 1970, 43, 713-720.	3.2	9
117	Photoionization electronic spectroscopy of AlNa. <i>Chemical Physics Letters</i> , 1994, 222, 353-357.	2.6	9
118	A theoretical study of Si <sub>4</sub> H <sub>2</sub> cluster with ab initio and density functional theory methods. <i>Journal of Chemical Physics</i> , 2001, 114, 1278-1285.	3.0	9
119	The single excitation perturbation expansion theory based on the locally projected molecular orbitals for molecular interaction: Comparison with the counterpoise corrected energy. <i>Chemical Physics Letters</i> , 2006, 431, 204-209.	2.6	9
120	Hydrogen-Bonded Networks in Hydride Water Clusters, F <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> and Cl <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> : Cubic Form of F <sup>+</sup> (H <sub>2</sub> O) <sub>7</sub> and Cl <sup>+</sup> (H <sub>2</sub> O) <sub>7</sub> . <i>Journal of Physical Chemistry A</i> , 2015, 119, 10241-10253.	2.5	9
121	Active reaction subsystem CI studies of peroxy free radicals aminoperoxy radical (H <sub>2</sub> NO <sub>2</sub> ). <i>Chemical Physics Letters</i> , 1980, 76, 375-379.	2.6	8
122	Absolutely Local Excited Orbitals in the Higher Order Perturbation Expansion for the Molecular Interaction. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16104-16109.	2.6	8
123	Electronic origin of the dependence of hydrogen bond strengths on nearest-neighbor and next-nearest-neighbor hydrogen bonds in polyhedral water clusters (H <sub>2</sub> O) <sub>n</sub> , n = 8, 20 and 24. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19746-19756.	2.8	8
124	Theoretical study of the three isomers of the SiNO radical. <i>Chemical Physics Letters</i> , 1992, 189, 401-407.	2.6	7
125	Accurate evaluation of Einstein's A and B coefficients of rovibrational transitions for carbon monoxide: spectral simulation of P <sup>v</sup> =2 rovibrational transitions in the solar atmosphere observed by a satellite. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2002, 72, 813-825.	2.3	7
126	2 Electronic and geometric structures of water cluster complexes with a group 1 metal atom: Electron-hydrogen bond in the OH <sub>e</sub> HO structure. <i>Advances in Metal and Semiconductor Clusters</i> , 2001, , 39-75.	1.5	7



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127	The excimer emission spectra and the interaction potential energy of the ground and excited states of He and alkali-metal ion systems. <i>Chemical Physics Letters</i> , 1992, 192, 443-450.	2.6	6
128	Theoretical studies of the new radicals SiNNH and SiCOH. <i>Chemical Physics Letters</i> , 1992, 195, 475-481.	2.6	5
129	Theoretical study on the non-adiabatic photodissociation process of argon cluster ions Ar7+. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 529-539.	2.0	5
130	On approximating electron repulsion integrals with linear combination of atomic-electron distributions. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1319-1324.	2.0	5
131	Theoretical studies on the molecular dependence of bond dissociation after core excitations II: CH3CO(CH2)nCN, n = 0-3. <i>Journal of Computational Chemistry</i> , 2003, 24, 1329-1335.	3.3	5
132	Theoretical emission spectra of NeAl+ and ArAl+ in the vacuum ultraviolet region. <i>Chemical Physics Letters</i> , 1988, 146, 275-279.	2.6	4
133	Theoretical Prediction of Intracluster Reactions of B+(H2O)2 and B+(H2O)3: Hybrid Procedure of Ab Initio MO Calculations and Monte Carlo Samplings. <i>Bulletin of the Chemical Society of Japan</i> , 1997, 70, 2619-2629.	3.2	4
134	Ab initio MO studies of Si4NO+ clusters. <i>Chemical Physics Letters</i> , 1997, 273, 337-344.	2.6	4
135	LOCALLY PROJECTED MOLECULAR ORBITAL THEORY FOR MOLECULAR INTERACTION WITH A HIGH-SPIN OPEN-SHELL MOLECULE. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 819-833.	1.8	4
136	Theoretical Studies of Group 1 Metal Complexes with Hydrogen Fluoride, M(HF)n, M = Li, Na, and K: A New Type of Electrideres. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7499-7503.	2.5	4
137	Electronic absorption bandwidths of negative ions of aromatic hydrocarbons. <i>Chemical Physics</i> , 1976, 13, 65-72.	1.9	3
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