Yuji Mochizuki

List of Publications by Year
in descending order

179	4,525	94415 37	138468 58
papers	citations	h-index	g-index

185	185	185	1959
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Collective residue interactions in trimer complexes of SARS-CoV-2 spike proteins analyzed by fragment molecular orbital method. Applied Physics Express, 2022, 15, 017001.	2.4	7
2	Variational quantum eigensolver simulations with the multireference unitary coupled cluster ansatz: a case study of the C_{2v} quasi-reaction pathway of beryllium insertion into a H₂ molecule. Physical Chemistry Chemical Physics, 2022, 24, 8439-8452.	2.8	11
3	Acceleration of Environmental Electrostatic Potential Using Cholesky Decomposition with Adaptive Metric (CDAM) for Fragment Molecular Orbital (FMO) Method. Bulletin of the Chemical Society of Japan, 2021, 94, 91-96.	3.2	1
4	The ABINIT-MP Program. , 2021, , 53-67.		10
5	Extension to Multiscale Simulations. , 2021, , 529-546.		0
6	Modeling of Solid and Surface. , 2021, , 407-424.		0
7	Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. Applied Physics Express, 2021, 14, 027003.	2.4	12
8	Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. RSC Advances, 2021, 11, 3272-3279.	3.6	20
9	Density-Matrix Based Scheme of Basis Selection for Linear Combination of Fragment Molecular Orbitals. Journal of the Physical Society of Japan, 2021, 90, 064301.	1.6	0
10	Dynamic Cooperativity of Ligandâ€“Residue Interactions Evaluated with the Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2021, 125, 6501-6512.	2.6	17
11	Fragment molecular orbital based interaction analyses on complexes between SARS-CoV-2 RBD variants and ACE2. Japanese Journal of Applied Physics, 2021, 60, 090901.	1.5	8
12	Interaction Analysis on the SARS-CoV-2 Spike Protein Receptor Binding Domain Using Visualization of the Interfacial Electrostatic Complementarity. Journal of Physical Chemistry Letters, 2021, 12, 11267-11272.	4.6	16
13	Development Status of ABINIT-MP in 2021. Journal of Computer Chemistry Japan, 2021, 20, 132-136.	0.1	2
14	Stabilization Mechanism for a Nonfibrillar Amyloid Î² Oligomer Based on Formation of a Hydrophobic Core Determined by Dissipative Particle Dynamics. ACS Chemical Neuroscience, 2020, 11, 385-394.	3.5	15
15	Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease â^' Inhibitor N3 Complex (PDB ID: 6LU7). Journal of Chemical Information and Modeling, 2020, 60, 3593-3602.	5.4	84
16	Selfâ€Degradable Lipidâ€like Materials Based on â€œHydrolysis accelerated by the intraâ€Particle Enrichment of Reactant (HyPER)â€• for Messenger RNA Delivery. Advanced Functional Materials, 2020, 30, 1910575.	14.9	65
17	Folding simulation of small proteins by dissipative particle dynamics (DPD) with non-empirical interaction parameters based on fragment molecular orbital calculations. Applied Physics Express, 2020, 13, 017002.	2.4	17
18	Fragmentation at sp 2 carbon atoms in fragment molecular orbital method. Journal of Computational Chemistry, 2020, 41, 1416-1420.	3.3	4

#	Article	IF	Citations
19	Ab Initio Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations of (NH3)32 Cluster: Effects of Electron Correlation. Bulletin of the Chemical Society of Japan, 2020, 93, 553-560.	3.2	1
20	Interaction Analyses between Calcite/Apatite and Peptides by Fragment Molecular Orbital Method. Journal of Computer Chemistry Japan, 2020, 19, 1-7.	0.1	1
21	Development Status of ABINIT-MP in 2020. Journal of Computer Chemistry Japan, 2020, 19, 142-145.	0.1	3
22	Cm³⁺/Eu³⁺induced structural, mechanistic and functional implications for calmodulin. Physical Chemistry Chemical Physics, 2019, 21, 21213-21222.	2.8	34
23	Destabilization of DNA through interstrand crosslinking by UO22+. Chemical Communications, 2019, 55, 2015-2018.	4.1	12
24	Interaction between calcite and adsorptive peptide analyzed by fragment molecular orbital method. Japanese Journal of Applied Physics, 2019, 58, 120906.	1.5	6
25	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. Journal of Physical Chemistry B, 2019, 123, 957-973.	2.6	46
26	Development of an Analysis Toolkit, AnalysisFMO, to Visualize Interaction Energies Generated by Fragment Molecular Orbital Calculations. Journal of Chemical Information and Modeling, 2019, 59, 25-30.	5.4	13
27	Current Status of ABINIT-MP Open Series. Journal of Computer Chemistry Japan, 2019, 18, 129-131.	0.1	5
28	Development of the Fragment Molecular Orbital Method for Calculating Nonlocal Excitations in Large Molecular Systems. Journal of Physical Chemistry A, 2018, 122, 3886-3898.	2.5	28
29	Fragment Molecular Orbital Based Parametrization Procedure for Mesoscopic Structure Prediction of Polymeric Materials. Journal of Physical Chemistry B, 2018, 122, 338-347.	2.6	20
30	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: Implementation and DNA Study. Journal of Physical Chemistry B, 2018, 122, 4457-4471.	2.6	35
31	Theoretical analyses on water cluster structures in polymer electrolyte membrane by using dissipative particle dynamics simulations with fragment molecular orbital based effective parameters. RSC Advances, 2018, 8, 34582-34595.	3.6	26
32	Formation Mechanism of Lipid Membrane and Vesicle Using Small Angle X-ray Scattering and Dissipative Particle Dynamics (DPD) Method. Journal of Computer Chemistry Japan, 2018, 17, 172-179.	0.1	6
33	Accuracy of Dimer-ES Approximation on Fragment Molecular Orbital (FMO) Method . Chem-Bio Informatics Journal, 2018, 18, 119-122.	0.3	0
34	Interaction between a Single-Stranded DNA and a Binding Protein Viewed by the Fragment Molecular Orbital Method. Bulletin of the Chemical Society of Japan, 2018, 91, 1596-1605.	3.2	7
35	RIâ€MP3 calculations of biomolecules based on the fragment molecular orbital method. Journal of Computational Chemistry, 2018, 39, 1970-1978.	3.3	6
36	An automated framework to evaluate effective interactionparameters for dissipative particle dynamics simulations basedon the fragment molecular orbital (FMO) method. Journal of Computer Chemistry Japan, 2018, 17, 102-109.	0.1	9

#	Article	IF	Citations
37	Application of TensorFlow to recognition of visualized results of fragment molecular orbital (FMO) calculations. Chem-Bio Informatics Journal, 2018, 18, 58-69.	0.3	6
38	Deeper Level Parallelization and Performance Evaluation ofFMO Program ABINIT-MP on Oakforest-PACS. Journal of Computer Chemistry Japan, 2018, 17, 147-149.	0.1	6
39	Fragment molecular orbital (FMO) calculations on DNA by a scaled third-order MÃller-Plesset perturbation (MP2.5) scheme. Computational and Theoretical Chemistry, 2017, 1101, 46-54.	2.5	15
40	Dissipative particle dynamics (DPD) simulations with fragment molecular orbital (FMO) based effective parameters for 1-Palmitoyl-2-oleoyl phosphatidyl choline (POPC) membrane. Chemical Physics Letters, 2017, 684, 427-432.	2.6	29
41	Explicit solvation of a single-stranded DNA, a binding protein,Âand their complex: a suitable protocol forÂfragment molecular orbital calculation. Chem-Bio Informatics Journal, 2017, 17, 72-84.	0.3	8
42	Current Status of ABINIT-MP as a FMO Program and Related Works with Machine Learning. Journal of Computer Chemistry Japan, 2017, 16, 119-122.	0.1	8
43	Development and Performance Evaluation of a Simulation Code for Dissipative Particle Dynamics (DPD) CAMUS. Journal of Computer Chemistry Japan, 2017, 16, 126-128.	0.1	2
44	A New Treatment for Water near the Interface between Lipid Membrane and Silica in Dissipative Particle Dynamics Simulation. Journal of Computer Chemistry Japan, 2017, 16, 28-31.	0.1	8
45	Theoretical Calculations on Cation-capturing ofMacrocyclic Peptoid with Phenyl Rings in Main Chain. Journal of Computer Chemistry Japan, 2017, 16, 77-79.	0.1	0
46	Performance Evaluations of Parallelized DFT Calculations with SMASH on Intel Xeon Phi Processor. Journal of Computer Chemistry Japan, 2016, 15, 92-96.	0.1	1
47	Hydration of ligands of influenza virus neuraminidase studied by the fragment molecular orbital method. Journal of Molecular Graphics and Modelling, 2016, 69, 144-153.	2.4	12
48	Fragment Molecular Orbital (FMO) Calculations of Peptoids. Journal of Computer Chemistry Japan, 2016, 15, 51-52.	0.1	3
49	Practical Usages Of 3D-printer for Scientific Education of Chemistry and Biology. Journal of Computer Chemistry Japan, 2016, 15, 66-67.	0.1	1
50	Fragment Molecular Orbital-Based Molecular Dynamics Study on Hydrated Ln(III) Ions. , 2015, , .		0
51	Explicit solvation modulates intra- and inter-molecular interactions within DNA: Electronic aspects revealed by the ab initio fragment molecular orbital (FMO) method. Computational and Theoretical Chemistry, 2015, 1054, 29-37.	2.5	20
52	Hydration effects on enzymeâ€“substrate complex of nylon oligomer hydrolase: inter-fragment interaction energy study by the fragment molecular orbital method. Molecular Physics, 2015, 113, 319-326.	1.7	6
53	Modeling of hydroxyapatiteâ€“peptide interaction based on fragment molecular orbital method. Chemical Physics Letters, 2015, 629, 58-64.	2.6	20
54	Implementation of Pair Interaction Energy DecompositionAnalysis and Its Applications to Protein-Ligand Systems. Journal of Computer Chemistry Japan, 2015, 14, 1-9.	0.1	40

#	Article	IF	Citations
55	Effects of Water Molecules and Configurations of Neighboring Amino Acid Residues Surrounding DsRed Chromophore on Its Excitation Energy. Journal of Computer Chemistry Japan, 2015, 14, 155-163.	0.1	0
56	Improved description of the orbital relaxation effect by practical use of the selfâ€energy. International Journal of Quantum Chemistry, 2014, 114, 577-586.	2.0	0
57	Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. Physical Chemistry Chemical Physics, 2014, 16, 10310-10344.	2.8	251
58	Interaction energy analysis on specific binding of influenza virus hemagglutinin to avian and human sialosaccharide receptors: Importance of mutation-induced structural change. Journal of Molecular Graphics and Modelling, 2014, 53, 48-58.	2.4	17
59	Accuracy of the fragment molecular orbital (FMO) calculations for DNA: Total energy, molecular orbital, and inter-fragment interaction energy. Computational and Theoretical Chemistry, 2014, 1034, 7-16.	2.5	16
60	Fragment molecular orbitalâ^'based molecular dynamics (FMO-MD) simulations on hydrated Cu(II) ion. Chem-Bio Informatics Journal, 2014, 14, 1-13.	0.3	5
61	Optimal damping algorithm for unrestricted Hartree-Fock calculations. Chem-Bio Informatics Journal, 2014, 14, 14-33.	0.3	1
62	Modeling of peptideâ€“silica interaction based on four-body corrected fragment molecular orbital (FMO4) calculations. Chemical Physics Letters, 2013, 566, 25-31.	2.6	30
63	Three- and four-body corrected fragment molecular orbital calculations with a novel subdividing fragmentation method applicable to structure-based drug design. Journal of Molecular Graphics and Modelling, 2013, 41, 31-42.	2.4	48
64	Dynamic fragmentation with static fragments (DF/SF) algorithm designed for ab initio fragment molecular orbital-based molecular dynamics (FMO-MD) simulations of polypeptides. Chem-Bio Informatics Journal, 2013, 13, 45-57.	0.3	1
65	Differences in hydration between cis- and trans-platin: Quantum insights by ab initio fragment molecular orbital-based molecular dynamics (FMO-MD). Computational and Theoretical Chemistry, 2012, 986, 30-34.	2.5	21
66	Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. Computational and Theoretical Chemistry, 2012, 997, 7-13.	2.5	10
67	Ab Initio Path Integral Molecular Dynamics and Monte Carlo Simulations for Water Trimer and Oligopeptide. ACS Symposium Series, 2012, , 187-199.	0.5	0
68	FMOâ€MD Simulations on the Hydration of Formaldehyde in Water Solution with Constraint Dynamics. Chemistry - A European Journal, 2012, 18, 9714-9721.	3.3	23
69	Development of the four-body corrected fragment molecular orbital (FMO4) method. Chemical Physics Letters, 2012, 523, 128-133.	2.6	56
70	Excited state calculation for free-base and metalloporphyrins with the partially renormalized polarization propagator approach. Chemical Physics Letters, 2012, 525-526, 144-149.	2.6	6
71	Partial geometry optimization with FMO-MP2 gradient: Application to TrpCage. Chemical Physics Letters, 2012, 535, 157-162.	2.6	18
72	Prediction of probable mutations in influenza virus hemagglutinin protein based on large-scale ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2011, 30, 110-119.	2.4	26

#	Article	IF	Citations
73	Higher-order correlated calculations based on fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2011, 130, 515-530.	1.4	78
74	Antigenâ€“antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. Theoretical Chemistry Accounts, 2011, 130, 1197-1202.	1.4	16
75	Fragment molecular orbital calculations for excitation energies of blue- and yellow-fluorescent proteins. Chemical Physics Letters, 2011, 504, 76-82.	2.6	16
76	Fragment molecular orbital-based molecular dynamics (FMO-MD) method with MP2 gradient. Chemical Physics Letters, 2011, 504, 95-99.	2.6	38
77	Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. Chemical Physics Letters, 2011, 509, 67-71.	2.6	24
78	4f-in-core model core potentials for trivalent lanthanides. Chemical Physics Letters, 2011, 510, 261-266.	2.6	13
79	1P260 Fragment molecular orbital calculation of the absorption maxima of bacteriorhodopsin and pharaonis phoborhodopsin(Photobiology:Vision & Photoreception,The 48th Annual Meeting of the) Tj ETQq1 1 0.784314 rgBT /Overlo	3.3	
80	Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. Chemical Physics Letters, 2010, 490, 84-89.	2.6	51
81	Does Amination of Formaldehyde Proceed Through a Zwitterionic Intermediate in Water? Fragment Molecular Orbital Molecular Dynamics Simulations by Using Constraint Dynamics. Chemistry - A European Journal, 2010, 16, 6430-6433.	3.3	21
82	Theoretical study of hydration models of trivalent rare-earth ions using model core potentials. Computational and Theoretical Chemistry, 2010, 949, 28-35.	1.5	26
83	Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA)â€“RNA complex system. Computational and Theoretical Chemistry, 2010, 962, 45-55.	1.5	18
84	Flexible ligand recognition of peroxisome proliferator-activated receptor-Î³ (PPARÎ³). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3344-3347.	2.2	21
85	Three-body expansion and generalized dynamic fragmentation improve the fragment molecular orbital-based molecular dynamics (FMO-MD). Chemical Physics Letters, 2010, 484, 380-386.	2.6	53
86	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion. Chemical Physics Letters, 2010, 490, 41-45.	2.6	35
87	Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). Chemical Physics Letters, 2010, 493, 346-352.	2.6	44
88	Theoretical Analysis of the Molecular Mechanism of Stabilization of Nova-RNA Complex System: Fragment Molecular Orbital Method Based Quantum Chemical Calculation For the Effect of the Complex Formation on the Electronic State of Biomacromolecular System. Biophysical Journal, 2010, 98, 74a.	0.5	0
89	Fragment Molecular Orbital methodâ€based Molecular Dynamics (FMOâ€MD) as a simulator for chemical reactions in explicit solvation. Journal of Computational Chemistry, 2009, 30, 40-50.	3.3	57
90	Fragment molecular orbital-based molecular dynamics (FMO-MD), a quantum simulation tool for large molecular systems. Computational and Theoretical Chemistry, 2009, 898, 2-7.	1.5	59

#	Article	IF	Citations
91	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. II. Towards an improvement of force fields used for classical molecular dynamics simulations. Chemical Physics Letters, 2009, 467, 417-423.	2.6	42
92	Application of Dyson-corrected second-order perturbation theories. Chemical Physics Letters, 2009, 472, 143-148.	2.6	8
93	Ab initio quantum-chemical study on emission spectra of bioluminescent luciferases by fragment molecular orbital method. Chemical Physics Letters, 2009, 472, 118-123.	2.6	39
94	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	2.6	41
95	Possibility of Mutation Prediction of Influenza Hemagglutinin by Combination of Hemadsorption Experiment and Quantum Chemical Calculation for Antibody Binding. Journal of Physical Chemistry B, 2009, 113, 4991-4994.	2.6	49
96	Fragment Molecular Orbital Calculations on Red Fluorescent Proteins (DsRed and mFruits). Journal of Physical Chemistry B, 2009, 113, 1153-1161.	2.6	40
97	2SP6-07 Possibility of Mutation Prediction of Influenza Hemagglutinin by Combination of Hemadsorption Experiment and Quantum Chemical Calculation for Antibody Binding(2SP6 Towards) Tj ETQq1 1 0.784314 rgBT /Ove	0.1	0
98	Developments of FMO Methodology and Graphical User Interface in ABINIT-MP. , 2009, , 37-62.		6
99	Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules. , 2009, , 133-170.		3
100	Excited States of Photoactive Proteins by Configuration Interaction Studies. , 2009, , 63-90.		0
101	Theoretical analysis of binding specificity of influenza viral hemagglutinin to avian and human receptors based on the fragment molecular orbital method. Computational Biology and Chemistry, 2008, 32, 198-211.	2.3	52
102	Multi-reference calculations of nitric oxide dimer. Chemical Physics Letters, 2008, 451, 31-36.	2.6	13
103	A practical use of self-energy shift for the description of orbital relaxation. Chemical Physics Letters, 2008, 453, 109-116.	2.6	14
104	Large scale FMO-MP2 calculations on a massively parallel-vector computer. Chemical Physics Letters, 2008, 457, 396-403.	2.6	113
105	An application of fragment interaction analysis based on local MP2. Chemical Physics Letters, 2008, 463, 189-194.	2.6	30
106	How Does an S_N2 Reaction Take Place in Solution? Full Ab Initio MD Simulations for the Hydrolysis of the Methyl Diazonium Ion. Journal of the American Chemical Society, 2008, 130, 2396-2397.	13.7	71
107	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions in Liganded Retinoid X Receptor: Specification of Residues Associated with Ligand Inducible Information Transmission. Journal of Physical Chemistry B, 2008, 112, 12081-12094.	2.6	47
108	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions between Liganded Retinoid X Receptor and Its Coactivator; Part II:â€‰ Influence of Mutations in Transcriptional Activation Function 2 Activating Domain Core on the Molecular Interactions. Journal of Physical Chemistry A, 2008, 112, 1986-1998.	2.5	37

#	Article	IF	Citations
109	Theoretical Study on Emission Spectra of Bioluminescent Luciferases by Fragment Molecular Orbital Method. Journal of Computer Aided Chemistry, 2008, 9, 47-54.	0.3	1
110	ON MECHANISM OF ENHANCED FLUORESCENCE IN GREEN FLUORESCENT PROTEIN. Biophysical Reviews and Letters, 2007, 02, 221-227.	0.8	2
111	Ab initio FMO-MD Method Reimplemented and Applied to Pure Water. AIP Conference Proceedings, 2007, , .	0.4	0
112	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions between Liganded Retinoid X Receptor and Its Coactivator:Â Roles of Helix 12 in the Coactivator Binding Mechanism. Journal of Physical Chemistry B, 2007, 111, 3525-3533.	2.6	33
113	Application of Fragment Molecular Orbital (FMO) Method to Nano-Bio Field. Journal of Computer Chemistry Japan, 2007, 6, 173-184.	0.1	1
114	Intra- and intermolecular interactions between cyclic-AMP receptor protein and DNA: Abinitio fragment molecular orbital study. Journal of Computational Chemistry, 2007, 28, 2237-2239.	3.3	3
115	Fragment molecular orbital calculations on red fluorescent protein (DsRed). Chemical Physics Letters, 2007, 433, 360-367.	2.6	33
116	A fully quantum mechanical simulation study on the lowest nâ€“Ï€â^— state of hydrated formaldehyde. Chemical Physics Letters, 2007, 437, 66-72.	2.6	52
117	Modification for spin-adapted version of configuration interaction singles with perturbative doubles. Chemical Physics Letters, 2007, 443, 389-397.	2.6	22
118	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. Chemical Physics Letters, 2007, 449, 329-335.	2.6	36
119	Visualization analysis of inter-fragment interaction energies of CRPâ€“cAMPâ€“DNA complex based on the fragment molecular orbital method. Biophysical Chemistry, 2007, 130, 1-9.	2.8	47
120	A graphical symmetric group approach for a spin adapted full configuration interaction: partitioning of a configuration graph into sets of closed-shell and open-shell graphs. Theoretical Chemistry Accounts, 2007, 117, 397-405.	1.4	8
121	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2007, 117, 541-553.	1.4	71
122	Fragment interaction analysis based on local MP2. Theoretical Chemistry Accounts, 2007, 118, 937-945.	1.4	62
123	Effects of Point Mutations on the Binding Energies of Estrogen Receptor with Estradiol. Journal of Computer Chemistry Japan, 2007, 6, 33-46.	0.1	2
124	Molecular Interactions between Estrogen Receptor and Its Ligand Studied by the ab Initio Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2006, 110, 16102-16110.	2.6	118
125	VISCANA:Â Visualized Cluster Analysis of Proteinâ^'Ligand Interaction Based on the ab Initio Fragment Molecular Orbital Method for Virtual Ligand Screening. Journal of Chemical Information and Modeling, 2006, 46, 221-230.	5.4	127
126	Dynamic polarizability calculation with fragment molecular orbital scheme. Chemical Physics Letters, 2006, 418, 418-422.	2.6	31

#	Article	IF	Citations
127	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	2.6	53
128	Application of fragment molecular orbital scheme to silicon-containing systems. Chemical Physics Letters, 2006, 430, 361-366.	2.6	15
129	Intra- and intermolecular interactions between cyclic-AMP receptor protein and DNA:Ab initio fragment molecular orbital study. Journal of Computational Chemistry, 2006, 27, 948-960.	3.3	107
130	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
131	Configuration interaction singles method with multilayer fragment molecular orbital scheme. Chemical Physics Letters, 2005, 406, 283-288.	2.6	112
132	A size-extensive modification of super-CI for orbital relaxation. Chemical Physics Letters, 2005, 410, 165-171.	2.6	12
133	A configuration analysis for fragment interaction. Chemical Physics Letters, 2005, 410, 247-253.	2.6	87
134	A parallelized integral-direct second-order Mï¿½ller?Plesset perturbation theory method with a fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2004, 112, 442-452.	1.4	160
135	Large scale MP2 calculations with fragment molecular orbital scheme. Chemical Physics Letters, 2004, 396, 473-479.	2.6	186
136	Comments on relativistic basis sets. Theoretical Chemistry Accounts, 2003, 109, 40-42.	1.4	22
137	On the electronic structures of Th4+ and Ac3+ hydrate models. Chemical Physics Letters, 2003, 372, 114-120.	2.6	14
138	Theoretical study of hydrolysis reactions of tetravalent thorium ion. Chemical Physics Letters, 2003, 373, 213-217.	2.6	8
139	Ab initio study on the structures of Th(IV) hydrate and its hydrolysis products in aqueous solution. Chemical Physics Letters, 2003, 375, 204-212.	2.6	44
140	Prolapses in four-component relativistic Gaussian basis sets. Chemical Physics Letters, 2003, 375, 399-405.	2.6	26
141	Comparative study of dehydrogenation of methanol at Pt(111)/water and Pt(111)/vacuum interfaces. Chemical Physics Letters, 2003, 377, 236-242.	2.6	58
142	On the electronic structure of CmFn (n=1â€“4) by all-electron Diracâ€“Hartreeâ€“Fock calculations. Journal of Chemical Physics, 2003, 118, 9201-9207.	3.0	8
143	On the electronic structure of Cm(H2O)n3+ (n=1,2,4,6) by all-electron Diracâ€“Hartreeâ€“Fock calculations. Journal of Chemical Physics, 2002, 116, 8838-8842.	3.0	18
144	Ab initio MO studies on the hydration of trivalent curium ion. Journal of Nuclear Science and Technology, 2002, 39, 418-421.	1.3	1

#	Article	IF	Citations
145	Size, Order, and Dimensional Relations for Silicon Cluster Polarizabilities. Journal of Physical Chemistry A, 2002, 106, 395-399.	2.5	20
146	Vectorization of Direct Fock Matrix Construction in DIRAC-DHF Calculations. Journal of Nuclear Science and Technology, 2002, 39, 195-199.	1.3	4
147	Four-component relativistic calculations on the mono-ammine complexes of trivalent f0, f7, and f14 ions. Chemical Physics Letters, 2002, 359, 331-336.	2.6	3
148	Vectorization of Direct Fock Matrix Construction in DIRAC-DHF Calculations.. Journal of Nuclear Science and Technology, 2002, 39, 195-199.	1.3	1
149	Vaporâ"Liquid Equilibrium Data for the Four Binary Systems Containing Fluorocarbon, Hydrofluorocarbon, and Fluorinated Ethers at 101.3 kPa. Journal of Chemical & Engineering Data, 2001, 46, 913-917.	1.9	22
150	Four-component relativistic calculations on the complexes between a water molecule and trivalent lanthanoid and actinoid ions. Chemical Physics, 2001, 273, 135-148.	1.9	24
151	HF-STEX and RASSCF calculations on nitrogenK-shell X-ray absorption of purine base and its derivative. Journal of Synchrotron Radiation, 2001, 8, 1003-1005.	2.4	14
152	Polarizability of silicon clusters. Chemical Physics Letters, 2001, 336, 451-456.	2.6	11
153	Modification of nonrelativistic Gaussian basis sets for relativistic calculations. Journal of Chemical Physics, 2001, 115, 9160-9164.	3.0	7
154	MULTI-REFERENCE COUPLED PAIR APPROXIMATION: a state-universal approach of a CEPA type variant of MRSDCI. Recent Advances in Computational, 1999, , 95-130.	0.8	4
155	A theoretical investigation of sulphur K-shell X-ray absorption of cysteine. Chemical Physics Letters, 1999, 309, 241-248.	2.6	17
156	Theoretical investigation of the GaF molecule and its positive ion. Theoretical Chemistry Accounts, 1999, 101, 257-261.	1.4	13
157	Theoretical spectroscopic constants of the GaN molecule. Theoretical Chemistry Accounts, 1999, 101, 292-296.	1.4	10
158	Multireference coupled-pair approximation study of the CuSi molecule. Theoretical Chemistry Accounts, 1999, 101, 332-335.	1.4	12
159	A CSF-based multi-reference coupled pair approximation. Theoretical Chemistry Accounts, 1998, 98, 165-170.	1.4	15
160	Theoretical investigation on the GaH molecule and its positive ion. Theoretical Chemistry Accounts, 1998, 99, 88-94.	1.4	18
161	Determination of valence band splitting parameters in GaN. Journal of Applied Physics, 1998, 83, 4542-4544.	2.5	49
162	Reflectance spectroscopy on GaN films under uniaxial stress. Applied Physics Letters, 1997, 71, 374-376.	3.3	31

#	Article	IF	Citations
163	Computational study of the spectroscopic constants of the ground state of the As2 molecule. Chemical Physics Letters, 1997, 274, 264-268.	2.6	9
164	Generalized doubly symbolic formulation for integral-driven direct configuration interaction method. Theoretica Chimica Acta, 1996, 93, 211-233.	0.8	4
165	Theoretical Study of the Surface Reaction Mechanism of GaN with HCl. Japanese Journal of Applied Physics, 1996, 35, L1641-L1643.	1.5	6
166	Theoretical study on the direct reaction between AsH3 and surface-adsorbed GaCl. Journal of Crystal Growth, 1995, 148, 96-105.	1.5	8
167	On the Reaction Scheme for Ti/TiN Chemical Vapor Deposition (CVD) Process Using TiCl4. Japanese Journal of Applied Physics, 1995, 34, L326-L329.	1.5	11
168	Theoretical study ofAs2desorption from the Ga dangling-bond site. Physical Review B, 1994, 49, 4658-4667.	3.2	11
169	Theoretical studies on the chloride ALE process. Applied Surface Science, 1994, 82-83, 200-207.	6.1	7
170	Theoretical study of the Cl desorption reaction induced by H2 in the chloride atomic layer epitaxy. Journal of Crystal Growth, 1994, 135, 259-268.	1.5	12
171	New Concerted Mechanism of the Cl-Removal Reaction Induced by H2in Chloride Atomic Layer Epitaxy. Japanese Journal of Applied Physics, 1993, 32, L197-L199.	1.5	10
172	Theoretical study of the gallium chloride molecule and its interaction with arsenic dangling bonds. Physical Review B, 1993, 47, 13420-13431.	3.2	9
173	Electronic structure of lower singlet states of binuclear copper acetate monohydrate. Canadian Journal of Chemistry, 1992, 70, 393-398.	1.1	8
174	Electronic structure of the linear form of OCuO. Chemical Physics, 1991, 151, 11-20.	1.9	21
175	A theoretical study of the CuOH molecule. Chemical Physics Letters, 1991, 185, 535-543.	2.6	12
176	Electronic structure of CO adsorbed on small Cu clusters: Theoretical study on excited states. Physical Review B, 1989, 39, 11907-11913.	3.2	8
177	A theoretical study of the bent form of CuO2. Chemical Physics Letters, 1989, 164, 225-230.	2.6	23
178	Ab initio cas SCF/MRSDCI study of the CuCH2 cluster. Chemical Physics Letters, 1988, 152, 457-463.	2.6	10
179	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations. , 0, , .		11