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	Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. Physical Chemistry Chemical Physics, 2014, 16, 10310-10344.	2.8	251
2	Large scale MP2 calculations with fragment molecular orbital scheme. Chemical Physics Letters, 2004, 396, 473-479.	2.6	186
3	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
4	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
5	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
6	Large scale FMO-MP2 calculations on a massively parallel-vector computer. Chemical Physics Letters, 2008, 457, 396-403.	2.6	113
7	Configuration interaction singles method with multilayer fragment molecular orbital scheme. Chemical Physics Letters, 2005, 406, 283-288.	2.6	112
8	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
9	A configuration analysis for fragment interaction. Chemical Physics Letters, 2005, 410, 247-253.	2.6	87
10	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
11	Higher-order correlated calculations based on fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2011, 130, 515-530.	1.4	78
12	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2007, 117, 541-553.	1.4	71
13	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
14	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
15	Fragment interaction analysis based on local MP2. Theoretical Chemistry Accounts, 2007, 118, 937-945.	1.4	62
16	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
17	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
18	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

#	Article	IF	Citations
19	Development of the four-body corrected fragment molecular orbital (FMO4) method. Chemical Physics Letters, 2012, 523, 128-133.	2.6	56
20	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	2.6	53
21	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
22	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
23	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
24	Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. Chemical Physics Letters, 2010, 490, 84-89.	2.6	51
25	Determination of valence band splitting parameters in GaN. Journal of Applied Physics, 1998, 83, 4542-4544.	2.5	49
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	2.6	41
35	Fragment Molecular Orbital Calculations on Red Fluorescent Proteins (DsRed and mFruits). Journal of Physical Chemistry B, 2009, 113, 1153-1161.	2.6	40
36	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

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37	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
38	Fragment molecular orbital-based molecular dynamics (FMO-MD) method with MP2 gradient. Chemical Physics Letters, 2011, 504, 95-99.	2.6	38
39	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
40	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. Chemical Physics Letters, 2007, 449, 329-335.	2.6	36
41	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
42	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion. Chemical Physics Letters, 2010, 490, 41-45.	2.6	35
43	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
44	Cm³⁺/Eu³⁺induced structural, mechanistic and functional implications for calmodulin. Physical Chemistry Chemical Physics, 2019, 21, 21213-21222.	2.8	34
45	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
46	Fragment molecular orbital calculations on red fluorescent protein (DsRed). Chemical Physics Letters, 2007, 433, 360-367.	2.6	33
47	Reflectance spectroscopy on GaN films under uniaxial stress. Applied Physics Letters, 1997, 71, 374-376.	3.3	31
48	Dynamic polarizability calculation with fragment molecular orbital scheme. Chemical Physics Letters, 2006, 418, 418-422.	2.6	31
49	An application of fragment interaction analysis based on local MP2. Chemical Physics Letters, 2008, 463, 189-194.	2.6	30
50	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
51	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
52	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
53	Prolapses in four-component relativistic Gaussian basis sets. Chemical Physics Letters, 2003, 375, 399-405.	2.6	26
54	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

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55	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
56	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
57	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
58	Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. Chemical Physics Letters, 2011, 509, 67-71.	2.6	24
59	A theoretical study of the bent form of CuO2. Chemical Physics Letters, 1989, 164, 225-230.	2.6	23
60	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
61	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
62	Comments on relativistic basis sets. Theoretical Chemistry Accounts, 2003, 109, 40-42.	1.4	22
63	Modification for spin-adapted version of configuration interaction singles with perturbative doubles. Chemical Physics Letters, 2007, 443, 389-397.	2.6	22
64	Electronic structure of the linear form of OCuO. Chemical Physics, 1991, 151, 11-20.	1.9	21
65	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
66	Flexible ligand recognition of peroxisome proliferator-activated receptor-Î³ (PPARÎ³). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3344-3347.	2.2	21
67	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
68	Size, Order, and Dimensional Relations for Silicon Cluster Polarizabilities. Journal of Physical Chemistry A, 2002, 106, 395-399.	2.5	20
69	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
70	Modeling of hydroxyapatiteâ€"peptide interaction based on fragment molecular orbital method. Chemical Physics Letters, 2015, 629, 58-64.	2.6	20
71	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
72	Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. RSC Advances, 2021, 11, 3272-3279.	3.6	20

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73	Theoretical investigation on the GaH molecule and its positive ion. Theoretical Chemistry Accounts, 1998, 99, 88-94.	1.4	18
74	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
75	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
76	Partial geometry optimization with FMO-MP2 gradient: Application to TrpCage. Chemical Physics Letters, 2012, 535, 157-162.	2.6	18
77	A theoretical investigation of sulphur K-shell X-ray absorption of cysteine. Chemical Physics Letters, 1999, 309, 241-248.	2.6	17
78	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
79	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
80	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
81	Antigenâ€“antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. Theoretical Chemistry Accounts, 2011, 130, 1197-1202.	1.4	16
82	Fragment molecular orbital calculations for excitation energies of blue- and yellow-fluorescent proteins. Chemical Physics Letters, 2011, 504, 76-82.	2.6	16
83	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
84	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
85	A CSF-based multi-reference coupled pair approximation. Theoretical Chemistry Accounts, 1998, 98, 165-170.	1.4	15
86	Application of fragment molecular orbital scheme to silicon-containing systems. Chemical Physics Letters, 2006, 430, 361-366.	2.6	15
87	Fragment molecular orbital (FMO) calculations on DNA by a scaled third-order MÃ¸ller-Plesset perturbation (MP2.5) scheme. Computational and Theoretical Chemistry, 2017, 1101, 46-54.	2.5	15
88	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
89	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
90	On the electronic structures of Th4+ and Ac3+ hydrate models. Chemical Physics Letters, 2003, 372, 114-120.	2.6	14

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91	A practical use of self-energy shift for the description of orbital relaxation. Chemical Physics Letters, 2008, 453, 109-116.	2.6	14
92	Theoretical investigation of the GaF molecule and its positive ion. Theoretical Chemistry Accounts, 1999, 101, 257-261.	1.4	13
93	Multi-reference calculations of nitric oxide dimer. Chemical Physics Letters, 2008, 451, 31-36.	2.6	13
94	4f-in-core model core potentials for trivalent lanthanides. Chemical Physics Letters, 2011, 510, 261-266.	2.6	13
95	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
96	A theoretical study of the CuOH molecule. Chemical Physics Letters, 1991, 185, 535-543.	2.6	12
97	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
98	Multireference coupled-pair approximation study of the CuSi molecule. Theoretical Chemistry Accounts, 1999, 101, 332-335.	1.4	12
99	A size-extensive modification of super-CI for orbital relaxation. Chemical Physics Letters, 2005, 410, 165-171.	2.6	12
100	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
101	Destabilization of DNA through interstrand crosslinking by UO22+. Chemical Communications, 2019, 55, 2015-2018.	4.1	12
102	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
103	Theoretical study ofAs2desorption from the Ga dangling-bond site. Physical Review B, 1994, 49, 4658-4667.	3.2	11
104	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
105	Polarizability of silicon clusters. Chemical Physics Letters, 2001, 336, 451-456.	2.6	11
106	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations. , 0, , .		11
107	Variational quantum eigensolver simulations with the multireference unitary coupled cluster ansatz: a case study of the C₂v</sub> quasi-reaction pathway of beryllium insertion into a H₂ molecule. Physical Chemistry Chemical Physics, 2022, 24, 8439-8452.	2.8	11
108	Ab initio cas SCF/MRSDCI study of the CuCH2 cluster. Chemical Physics Letters, 1988, 152, 457-463.	2.6	10

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109	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
110	Theoretical spectroscopic constants of the GaN molecule. Theoretical Chemistry Accounts, 1999, 101, 292-296.	1.4	10
111	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
112	The ABINIT-MP Program. , 2021, , 53-67.		10
113	Theoretical study of the gallium chloride molecule and its interaction with arsenic dangling bonds. Physical Review B, 1993, 47, 13420-13431.	3.2	9
114	Computational study of the spectroscopic constants of the ground state of the As2 molecule. Chemical Physics Letters, 1997, 274, 264-268.	2.6	9
115	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
116	Electronic structure of CO adsorbed on small Cu clusters: Theoretical study on excited states. Physical Review B, 1989, 39, 11907-11913.	3.2	8
117	Electronic structure of lower singlet states of binuclear copper acetate monohydrate. Canadian Journal of Chemistry, 1992, 70, 393-398.	1.1	8
118	Theoretical study on the direct reaction between AsH3 and surface-adsorbed GaCl. Journal of Crystal Growth, 1995, 148, 96-105.	1.5	8
119	Theoretical study of hydrolysis reactions of tetravalent thorium ion. Chemical Physics Letters, 2003, 373, 213-217.	2.6	8
120	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
121	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
122	Application of Dyson-corrected second-order perturbation theories. Chemical Physics Letters, 2009, 472, 143-148.	2.6	8
123	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
124	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
125	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
126	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

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127	Theoretical studies on the chloride ALE process. Applied Surface Science, 1994, 82-83, 200-207.	6.1	7
128	Modification of nonrelativistic Gaussian basis sets for relativistic calculations. Journal of Chemical Physics, 2001, 115, 9160-9164.	3.0	7
129	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
130	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
131	Theoretical Study of the Surface Reaction Mechanism of GaN with HCl. Japanese Journal of Applied Physics, 1996, 35, L1641-L1643.	1.5	6
132	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
133	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
134	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
135	RIâ€MP3 calculations of biomolecules based on the fragment molecular orbital method. Journal of Computational Chemistry, 2018, 39, 1970-1978.	3.3	6
136	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
137	Interaction between calcite and adsorptive peptide analyzed by fragment molecular orbital method. Japanese Journal of Applied Physics, 2019, 58, 120906.	1.5	6
138	Developments of FMO Methodology and Graphical User Interface in ABINIT-MP. , 2009, , 37-62.		6
139	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
140	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
141	Current Status of ABINIT-MP Open Series. Journal of Computer Chemistry Japan, 2019, 18, 129-131.	0.1	5
142	Generalized doubly symbolic formulation for integral-driven direct configuration interaction method. Theoretica Chimica Acta, 1996, 93, 211-233.	0.8	4
143	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
144	Vectorization of Direct Fock Matrix Construction in DIRAC-DHF Calculations. Journal of Nuclear Science and Technology, 2002, 39, 195-199.	1.3	4

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145	Fragmentation at sp 2 carbon atoms in fragment molecular orbital method. Journal of Computational Chemistry, 2020, 41, 1416-1420.	3.3	4
146	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
147	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
148	Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules. , 2009, , 133-170.		3
149	Fragment Molecular Orbital (FMO) Calculations of Peptoids. Journal of Computer Chemistry Japan, 2016, 15, 51-52.	0.1	3
150	Development Status of ABINIT-MP in 2020. Journal of Computer Chemistry Japan, 2020, 19, 142-145.	0.1	3
151	ON MECHANISM OF ENHANCED FLUORESCENCE IN GREEN FLUORESCENT PROTEIN. Biophysical Reviews and Letters, 2007, 02, 221-227.	0.8	2
152	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
153	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
154	Development Status of ABINIT-MP in 2021. Journal of Computer Chemistry Japan, 2021, 20, 132-136.	0.1	2
155	Ab initio MO studies on the hydration of trivalent curium ion. Journal of Nuclear Science and Technology, 2002, 39, 418-421.	1.3	1
156	Application of Fragment Molecular Orbital (FMO) Method to Nano-Bio Field. Journal of Computer Chemistry Japan, 2007, 6, 173-184.	0.1	1
157	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
158	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
159	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
160	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
161	Optimal damping algorithm for unrestricted Hartree-Fock calculations. Chem-Bio Informatics Journal, 2014, 14, 14-33.	0.3	1
162	Interaction Analyses between Calcite/Apatite and Peptides by Fragment Molecular Orbital Method. Journal of Computer Chemistry Japan, 2020, 19, 1-7.	0.1	1

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163	Vectorization of Direct Fock Matrix Construction in DIRAC-DHF Calculations.. Journal of Nuclear Science and Technology, 2002, 39, 195-199.	1.3	1
164	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
165	Practical Usages Of 3D-printer for Scientific Education of Chemistry and Biology. Journal of Computer Chemistry Japan, 2016, 15, 66-67.	0.1	1
166	Ab initio FMO-MD Method Reimplemented and Applied to Pure Water. AIP Conference Proceedings, 2007, , .	0.4	0
167	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 /Over	0.1	0
168	1P260 Fragment molecular orbital calculation of the absorption maxima of bacteriorhodopsin and pharaonis phoborhodopsin(Photobiology:Vision & Photoreception,The 48th Annual Meeting of the) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5		0
169	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
170	Ab Initio Path Integral Molecular Dynamics and Monte Carlo Simulations for Water Trimer and Oligopeptide. ACS Symposium Series, 2012, , 187-199.	0.5	0
171	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
172	Fragment Molecular Orbital-Based Molecular Dynamics Study on Hydrated Ln(III) Ions. , 2015, , .		0
173	Accuracy of Dimer-ES Approximation on Fragment Molecular Orbital (FMO) Method . Chem-Bio Informatics Journal, 2018, 18, 119-122.	0.3	0
174	Extension to Multiscale Simulations. , 2021, , 529-546.		0
175	Modeling of Solid and Surface. , 2021, , 407-424.		0
176	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
177	Excited States of Photoactive Proteins by Configuration Interaction Studies. , 2009, , 63-90.		0
178	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
179	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