Yuto Komeiji

List of Publications by Year
in descending order

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73	2,108	279798	233421
papers	citations	23 h-index	45 g-index

79	79	79	1141
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	Fragment molecular orbital method: analytical energy gradients. Chemical Physics Letters, 2001, 336, 163-170.	2.6	197
3	Fragment molecular orbital method: application to molecular dynamics simulation, â€˜ab initio FMO-MDâ€™. Chemical Physics Letters, 2003, 372, 342-347.	2.6	112
4	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
5	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
6	Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer. Journal of Computational Chemistry, 1997, 18, 1546-1563.	3.3	75
7	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
8	Change in a protein's electronic structure induced by an explicit solvent: Anab initio fragment molecular orbital study of ubiquitin. Journal of Computational Chemistry, 2007, 28, 1750-1762.	3.3	69
9	Computational Observation of an Ion Permeation Through a Channel Protein. Bioscience Reports, 1998, 18, 39-48.	2.4	61
10	Molecular dynamics simulations revealed Ca2+ -dependent conformational change of Calmodulin. FEBS Letters, 2002, 521, 133-139.	2.8	59
11	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
12	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
13	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	2.6	53
14	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
15	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
16	A molecular dynamics study of solvent behavior around a protein. Proteins: Structure, Function and Bioinformatics, 1993, 16, 268-277.	2.6	51
17	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
18	PEACH 4 with ABINIT-MP: a general platform for classical and quantum simulations of biological molecules. Computational Biology and Chemistry, 2004, 28, 155-161.	2.3	45

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19	Ab initio fragment molecular orbital (FMO) method applied to analysis of the ligandâ€“protein interaction in a pheromone-binding protein. Computational Biology and Chemistry, 2005, 29, 434-439.	2.3	40
20	Fragment molecular orbital-based molecular dynamics (FMO-MD) method with MP2 gradient. Chemical Physics Letters, 2011, 504, 95-99.	2.6	38
21	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion. Chemical Physics Letters, 2010, 490, 41-45.	2.6	35
22	Cm³⁺/Eu³⁺induced structural, mechanistic and functional implications for calmodulin. Physical Chemistry Chemical Physics, 2019, 21, 21213-21222.	2.8	34
23	Molecular dynamics simulation of trp-aporepressor in a solvent. Protein Engineering, Design and Selection, 1991, 4, 871-875.	2.1	23
24	Molecular dynamics simulations oftrp apo-and holorepressors: Domain structure and ligand-protein interaction. Proteins: Structure, Function and Bioinformatics, 1994, 20, 248-258.	2.6	23
25	Parallel molecular dynamics simulation of a protein. Parallel Computing, 2001, 27, 977-987.	2.1	23
26	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
27	Ewald summation and multiple time step methods for molecular dynamics simulation of biological molecules. Computational and Theoretical Chemistry, 2000, 530, 237-243.	1.5	22
28	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
29	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
30	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
31	Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. RSC Advances, 2021, 11, 3272-3279.	3.6	20
32	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
33	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
34	Orientation of the carboxyl terminus of the Na+ /proline symport carrier in Escherichia coll. FEBS Letters, 1989, 256, 135-138.	2.8	15
35	Change in Conformation by DNA-Peptide Association: Molecular Dynamics of the Hin-Recombinaseâ€“ hixL Complex. Biophysical Journal, 1999, 77, 123-138.	0.5	15
36	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

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37	Molecular dynamics simulation of trp-repressor/operator complex: analysis of hydrogen bond patterns of proteinâ€“DNA interaction. Journal of Molecular Structure, 2000, 526, 209-218.	3.6	14
38	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
39	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
40	Glycine 85 of the trp-repressor of E.coli is important in forming the hydrophobic tryptophan binding pocket: experimental and computational approaches. Protein Engineering, Design and Selection, 1994, 7, 1239-1247.	2.1	11
41	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations. , 0, , .		11
42	Molecular Dynamics Simulation of the Hin-Recombinaseâ€”DNA Complex. Molecular Simulation, 1999, 21, 303-324.	2.0	10
43	Implementation of the blue moon ensemble method. Chem-Bio Informatics Journal, 2007, 7, 12-23.	0.3	10
44	The ABINIT-MP Program. , 2021, , 53-67.		10
45	Free energy perturbation study on a Trp-binding mutant (Ser88 â†’Cys) of the trp-repressor. Protein Engineering, Design and Selection, 1992, 5, 759-767.	2.1	8
46	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
47	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
48	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
49	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
50	Taking Water into Account with the Fragment Molecular Orbital Method. Methods in Molecular Biology, 2020, 2114, 105-122.	0.9	7
51	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
52	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
53	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
54	Flexibility of a loop in a pheromone binding protein from <I>Bombyx mori</I>: a molecular dynamics simulation. Chem-Bio Informatics Journal, 2002, 2, 32-37.	0.3	5

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55	Computational design of a substrate specificity mutant of a protein. , 1996, 26, 459-464.		4
56	Ca2+-ATPase Molecules as a Calcium-Sensitive Membrane-Endoskeleton of Sarcoplasmic Reticulum. International Journal of Molecular Sciences, 2021, 22, 2624.	4.1	4
57	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
58	Corrigendum to: Molecular dynamics simulations revealed Ca2+-dependent conformational change of Calmodulin (FEBS 26172). FEBS Letters, 2002, 523, 256-256.	2.8	2
59	Helix propensity of Ala and Val: A free energy perturbation study. Biophysical Chemistry, 1993, 47, 113-121.	2.8	1
60	Water-mediated interactions in the CRPâ€“cAMPâ€“DNA complex: Does water mediate sequence-specific binding at the DNA primary-kink site?. Computational Biology and Chemistry, 2008, 32, 149-158.	2.3	1
61	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
62	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
63	FMO Interfaced with Molecular Dynamics Simulation. , 2021, , 373-389.		1
64	Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer. , 1997, 18, 1546.		1
65	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
66	Peach-Grape system-a high performance simulator for biomolecules. Chem-Bio Informatics Journal, 2002, 2, 102-118.	0.3	1
67	Threonine 81 of the trp repressor of Escherichia coli plays an auxiliary role in the formation of the corepressor binding pocket. Protein Engineering, Design and Selection, 1995, 8, 935-938.	2.1	0
68	Ab initio FMO-MD Method Reimplemented and Applied to Pure Water. AIP Conference Proceedings, 2007, , .	0.4	0
69	Three-Body Expansion and Generalized Dynamic Fragmentation Improve the Fragment Molecular Orbital-Based Molecular Dynamics (fMO-MD), An ab Initio MD Method. Biophysical Journal, 2010, 98, 573a.	0.5	0
70	Fragment Molecular Orbital-Based Molecular Dynamics Study on Hydrated Ln(III) Ions. , 2015, , .		0
71	Accuracy of Dimer-ES Approximation on Fragment Molecular Orbital (FMO) Method . Chem-Bio Informatics Journal, 2018, 18, 119-122.	0.3	0
72	Potentiating Antigen-Specific Antibody Production with Peptides Obtained from In Silico Screening for High-Affinity against MHC-II. Molecules, 2019, 24, 2949.	3.8	0

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73	Fmo-Md. , 2009, , 119-131.		0