Shigenori Tanaka

List of Publications by Year
in descending order

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147	3,761	94381	175177
papers	citations	37 h-index	52 g-index

162	162	162	1784
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.	1.3	251
2	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.	1.2	118
3	Large scale FMO-MP2 calculations on a massively parallel-vector computer. Chemical Physics Letters, 2008, 457, 396-403.	1.2	113
4	Thermodynamics and Correlational Properties of Finite-Temperature Electron Liquids in the Singwi-Tosi-Land-SjÃ¶lander Approximation. Journal of the Physical Society of Japan, 1986, 55, 2278-2289.	0.7	112
5	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.	1.5	107
6	A configuration analysis for fragment interaction. Chemical Physics Letters, 2005, 410, 247-253.	1.2	87
7	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.	2.5	84
8	Higher-order correlated calculations based on fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2011, 130, 515-530.	0.5	78
9	Generalized viscoelastic theory of the glass transition for strongly coupled, classical, one-component plasmas. Physical Review Letters, 1986, 56, 2815-2818.	2.9	75
10	Fragment interaction analysis based on local MP2. Theoretical Chemistry Accounts, 2007, 118, 937-945.	0.5	62
11	Development of the four-body corrected fragment molecular orbital (FMO4) method. Chemical Physics Letters, 2012, 523, 128-133.	1.2	56
12	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	1.2	53
13	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.	1.1	52
14	Spin-dependent correlations and thermodynamic functions for electron liquids at arbitrary degeneracy and spin polarization. Physical Review B, 1989, 39, 1036-1051.	1.1	51
15	Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. Chemical Physics Letters, 2010, 490, 84-89.	1.2	51
16	Parametrized equation of state for electron liquids in the Singwi-Tosi-Land-SjÃ¶lander approximation. Physical Review A, 1985, 32, 1896-1899.	1.0	50
17	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.	1.2	49
18	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.	1.3	48

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19	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.	1.5	47
20	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.	1.2	47
21	Incorporation of solvation effects into the fragment molecular orbital calculations with the Poissonâ€“Boltzmann equation. Chemical Physics Letters, 2010, 500, 116-119.	1.2	47
22	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.	1.2	46
23	Effective Static Approximation: A Fast and Reliable Tool for Warm-Dense Matter Theory. Physical Review Letters, 2020, 125, 235001.	2.9	46
24	Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). Chemical Physics Letters, 2010, 493, 346-352.	1.2	44
25	Dynamic theory of correlations in strongly coupled, classical one-component plasmas: Glass transition in the generalized viscoelastic formalism. Physical Review A, 1987, 35, 4743-4754.	1.0	43
26	DNA and Estrogen Receptor Interaction Revealed by Fragment Molecular Orbital Calculations. Journal of Physical Chemistry B, 2007, 111, 9621-9627.	1.2	43
27	AutoDock-GIST: Incorporating Thermodynamics of Active-Site Water into Scoring Function for Accurate Protein-Ligand Docking. Molecules, 2016, 21, 1604.	1.7	43
28	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.	1.2	42
29	Electron Transfer Model for the Electric Field Effect on Quantum Yield of Charge Separation in Bacterial Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 1997, 101, 5031-5045.	1.2	41
30	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	1.2	41
31	Fragment molecular orbital calculations under periodic boundary condition. Chemical Physics Letters, 2011, 506, 112-116.	1.2	41
32	Theoretical Analysis of Activity Cliffs among Benzofuranone-Class Pim1 Inhibitors Using the Fragment Molecular Orbital Method with Molecular Mechanics Poissonâ€“Boltzmann Surface Area (FMO+MM-PBSA) Approach. Journal of Chemical Information and Modeling, 2017, 57, 2996-3010.	2.5	41
33	Fragment Molecular Orbital Calculations on Red Fluorescent Proteins (DsRed and mFruits). Journal of Physical Chemistry B, 2009, 113, 1153-1161.	1.2	40
34	Statistical correction to effective interactions in the fragment molecular orbital method. Chemical Physics Letters, 2013, 556, 272-277.	1.2	40
35	Ab initio quantum-chemical study on emission spectra of bioluminescent luciferases by fragment molecular orbital method. Chemical Physics Letters, 2009, 472, 118-123.	1.2	39
36	Strongly coupled electron liquid: Ab initio path integral Monte Carlo simulations and dielectric theories. Physical Review B, 2020, 101, .	1.1	38

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37	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.	1.1	37
38	Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses. Chemical Science, 2021, 12, 4722-4739.	3.7	37
39	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. Chemical Physics Letters, 2007, 449, 329-335.	1.2	36
40	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
41	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.	1.2	35
42	Correlational and thermodynamic properties of finite-temperature electron liquids in the hypernetted-chain approximation. Journal of Chemical Physics, 2016, 145, 214104.	1.2	34
43	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.	1.2	33
44	Fragment molecular orbital calculations on red fluorescent protein (DsRed). Chemical Physics Letters, 2007, 433, 360-367.	1.2	33
45	Dynamic polarizability calculation with fragment molecular orbital scheme. Chemical Physics Letters, 2006, 418, 418-422.	1.2	31
46	An application of fragment interaction analysis based on local MP2. Chemical Physics Letters, 2008, 463, 189-194.	1.2	30
47	Modeling of peptideâ€“silica interaction based on four-body corrected fragment molecular orbital (FMO4) calculations. Chemical Physics Letters, 2013, 566, 25-31.	1.2	30
48	Thermodynamic properties of water molecules in the presence of cosolute depend on DNA structure: a study using grid inhomogeneous solvation theory. Nucleic Acids Research, 2015, 43, gkv1133.	6.5	29
49	Fragment Molecular Orbital (FMO) and FMO-MO Calculations of DNA: Accuracy Validation of Energy and Interfragment Interaction Energy. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1328-1337.	0.4	26
50	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.	1.3	26
51	Cosolvent-Based Molecular Dynamics for Ensemble Docking: Practical Method for Generating Druggable Protein Conformations. Journal of Chemical Information and Modeling, 2017, 57, 742-756.	2.5	26
52	Development of an automated fragment molecular orbital (FMO) calculation protocol toward construction of quantum mechanical calculation database for large biomolecules . Chem-Bio Informatics Journal, 2019, 19, 5-18.	0.1	26
53	Roles of K151 and D180 in <scp>L</scp>â€2â€haloacid dehalogenase from Pseudomonas sp. YL: Analysis by molecular dynamics and ab initio fragment molecular orbital calculations. Journal of Computational Chemistry, 2009, 30, 2625-2634.	1.5	25
54	Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. Chemical Physics Letters, 2011, 509, 67-71.	1.2	24

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55	FMODB: The Worldâ€™s First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method. Journal of Chemical Information and Modeling, 2021, 61, 777-794.	2.5	24
56	Charge Clamps of Lysines and Hydrogen Bonds Play Key Roles in the Mechanism to Fix Helix 12 in the Agonist and Antagonist Positions of Estrogen Receptor Î±: Intramolecular Interactions Studied by the Ab Initio Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2014, 118, 4993-5008.	1.2	23
57	Newly characterized interaction stabilizes DNA structure: oligoethylene glycols stabilize G-quadruplexes CHâ€“Î€ interactions. Nucleic Acids Research, 2017, 45, 7021-7030.	6.5	23
58	Effects of salt addition on strength and dynamics of hydrophobic interactions. Chemical Physics Letters, 2007, 434, 42-48.	1.2	22
59	Ab initioPath Integral Molecular Dynamics Based on Fragment Molecular Orbital Method. Journal of the Physical Society of Japan, 2009, 78, 104723.	0.7	22
60	Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening. Computational and Theoretical Chemistry, 2018, 1132, 23-34.	1.1	22
61	Towards good correlation between fragment molecular orbital interaction energies and experimental IC50 for ligand binding: A case study of p38 MAP kinase. Computational and Structural Biotechnology Journal, 2018, 16, 421-434.	1.9	22
62	Proteinâ€“ligand docking using fitness learning-based artificial bee colony with proximity stimuli. Physical Chemistry Chemical Physics, 2015, 17, 16412-16417.	1.3	21
63	Computational Analysis of the Interaction Energies between Amino Acid Residues of the Measles Virus Hemagglutinin and Its Receptors. Viruses, 2018, 10, 236.	1.5	21
64	Fragment molecular orbital calculations for biomolecules. Current Opinion in Structural Biology, 2022, 72, 127-134.	2.6	21
65	Ion-Density Correlations and Enhancement of Thermonuclear Reaction Rate in Dense, Inertially Confined Fusion Plasmas. Journal of the Physical Society of Japan, 1984, 53, 2039-2048.	0.7	20
66	Stopping Power of Degenerate Electron Liquid at Metallic Densities. Journal of the Physical Society of Japan, 1985, 54, 2537-2542.	0.7	20
67	Nuclear quantum effects on electron transfer reactions in DNA hairpins. Physical Review E, 2003, 68, 031905.	0.8	20
68	DENSITY FUNCTIONAL CALCULATIONS ON THE INTERACTION BETWEEN CATABOLITE ACTIVATOR PROTEIN AND CYCLIC AMP USING THE FRAGMENT MOLECULAR ORBITAL METHOD. Journal of Theoretical and Computational Chemistry, 2005, 04, 183-195.	1.8	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.	1.1	20
70	Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. RSC Advances, 2021, 11, 3272-3279.	1.7	20
71	Theory of interparticle correlations in dense, high-temperature plasmas. VIII. Shear viscosity. Physical Review A, 1986, 34, 4163-4170.	1.0	19
72	Novel type of virtual ligand screening on the basis of quantum-chemical calculations for proteinâ€“ligand complexes and extended clustering techniques. Computational and Theoretical Chemistry, 2015, 1061, 12-22.	1.1	19

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73	Improved equation of state for finiteâ€temperature spinâ€polarized electron liquids on the basis of Singwiâ€“Tosiâ€“Landâ€“SjÃ¶lander approximation. Contributions To Plasma Physics, 2017, 57, 126-136.	0.5	19
74	ATP Converts Aî²₄₂ Oligomer into Off-Pathway Species by Making Contact with Its Backbone Atoms Using Hydrophobic Adenosine. Journal of Physical Chemistry B, 2019, 123, 9922-9933.	1.2	19
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	Affinity of Molecular Ions for DNA Structures Is Determined by Solvent-Accessible Surface Area. Journal of Physical Chemistry B, 2014, 118, 9583-9594.	1.2	18
77	Comparative Characterization of Short Monomeric Polyglutamine Peptides by Replica Exchange Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2010, 114, 7056-7061.	1.2	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.	1.3	17
79	Dynamic Cooperativity of Ligandâ€“Residue Interactions Evaluated with the Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2021, 125, 6501-6512.	1.2	17
80	Theory of nonadiabatic electron transfer at electrode/liquid interfaces: Role of quantum effects. Journal of Chemical Physics, 1999, 111, 11117-11137.	1.2	16
81	Fragmentation Method Combined with Quantum Monte Carlo Calculations. Journal of the Physical Society of Japan, 2007, 76, 064301.	0.7	16
82	Antigenâ€“antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. Theoretical Chemistry Accounts, 2011, 130, 1197-1202.	0.5	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.	1.1	16
84	Application of fragment molecular orbital scheme to silicon-containing systems. Chemical Physics Letters, 2006, 430, 361-366.	1.2	15
85	Sialic Acid Recognition of the Pandemic Influenza 2009 H1N1 Virus: Binding Mechanism Between Human Receptor and Influenza Hemagglutinin. Protein and Peptide Letters, 2011, 18, 530-539.	0.4	15
86	Study of the aggregation mechanism of polyglutamine peptides using replica exchange molecular dynamics simulations. Journal of Molecular Modeling, 2013, 19, 1627-1639.	0.8	15
87	Identification of correlated inter-residue interactions in protein complex based on the fragment molecular orbital method. Journal of Molecular Graphics and Modelling, 2020, 100, 107650.	1.3	15
88	Meteorite Impact-Induced Rapid NH3 Production on Early Earth: Ab Initio Molecular Dynamics Simulation. Scientific Reports, 2016, 6, 38953.	1.6	14
89	Local thermodynamics of the water molecules around single- and double-stranded DNA studied by grid inhomogeneous solvation theory. Chemical Physics Letters, 2016, 660, 250-255.	1.2	12
90	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.	1.1	12

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91	Ab initio study of molecular interactions in higher plant and Galdieria partita Rubiscos with the fragment molecular orbital method. Biochemical and Biophysical Research Communications, 2007, 361, 367-372.	1.0	10
92	Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. Computational and Theoretical Chemistry, 2012, 997, 7-13.	1.1	10
93	The ABINIT-MP Program. , 2021, , 53-67.		10
94	Proteinâ€“ligand binding affinity prediction of cyclinâ€dependent kinaseâ€2 inhibitors by dynamically averaged fragment molecular orbitalâ€based interaction energy. Journal of Computational Chemistry, 2022, 43, 1362-1371.	1.5	10
95	Molecular mechanics and all-electron fragment molecular orbital calculations on mutated polyglutamine peptides. Computational and Theoretical Chemistry, 2010, 944, 12-20.	1.5	9
96	Analysis of electron-transfer rate constant in condensed media with inclusion of inelastic tunneling and nuclear quantum effects. Physical Review E, 2010, 81, 027101.	0.8	9
97	Comparison of binding affinity evaluations for FKBP ligands with state-of-the-art computational methods: FMO, QM/MM, MM-PB/SA and MP-CAFEE approaches. Chem-Bio Informatics Journal, 2010, 10, 32-45.	0.1	9
98	Statistical-Mechanical Theory of Cold Nuclear Fusion in Metal Hydrides. Journal of the Physical Society of Japan, 1990, 59, 1333-1340.	0.7	8
99	Modulation of excitation energy transfer by conformational oscillations in biomolecular systems. Chemical Physics Letters, 2011, 508, 139-143.	1.2	8
100	A significant role of Arg41 residue in the enzymatic reaction of haloacid dehalogenase l-DEX YL studied by QM/MM method. Journal of Molecular Catalysis B: Enzymatic, 2014, 110, 23-31.	1.8	8
101	Current Status of ABINIT-MP as a FMO Program and Related Works with Machine Learning. Journal of Computer Chemistry Japan, 2017, 16, 119-122.	0.0	8
102	Comparative study on model parameter evaluations for the energy transfer dynamics in Fennaâ€“Matthewsâ€“Olson complex. Chemical Physics, 2020, 539, 110903.	0.9	8
103	Fragment molecular orbital based interaction analyses on complexes between SARS-CoV-2 RBD variants and ACE2. Japanese Journal of Applied Physics, 2021, 60, 090901.	0.8	8
104	Taking Water into Account with the Fragment Molecular Orbital Method. Methods in Molecular Biology, 2020, 2114, 105-122.	0.4	7
105	Collective residue interactions in trimer complexes of SARS-CoV-2 spike proteins analyzed by fragment molecular orbital method. Applied Physics Express, 2022, 15, 017001.	1.1	7
106	Classical density functional calculation of radial distribution functions of liquid water. Chemical Physics, 2014, 430, 18-22.	0.9	6
107	Theoretical prediction and experimental verification on enantioselectivity of haloacid dehalogenase l-DEX YL with chloropropionate. Chemical Physics Letters, 2015, 623, 101-107.	1.2	6
108	Systems approach to excitation-energy and electron transfer reaction networks in photosystem II complex: model studies for chlorophyll a fluorescence induction kinetics. Journal of Theoretical Biology, 2015, 380, 220-237.	0.8	6

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109	Structural transition of solvated H-Ras/GTP revealed by molecular dynamics simulation and local network entropy. Journal of Molecular Graphics and Modelling, 2017, 77, 51-63.	1.3	6
110	Reaction Pathway Sampling and Free-Energy Analyses for Multimeric Protein Complex Disassembly by Employing Hybrid Configuration Bias Monte Carlo/Molecular Dynamics Simulation. ACS Omega, 2021, 6, 4749-4758.	1.6	6
111	Reduced minimum model for the photosynthetic induction processes in photosystem I. Journal of Photochemistry and Photobiology B: Biology, 2016, 160, 364-375.	1.7	5
112	Meteorite impacts on ancient oceans opened up multiple NH₃ production pathways. Physical Chemistry Chemical Physics, 2017, 19, 11655-11667.	1.3	5
113	Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. Journal of Computational Chemistry, 2019, 40, 349-359.	1.5	5
114	New Modified Deoxythymine with Dibranched Tetraethylene Glycol Stabilizes G-Quadruplex Structures. Molecules, 2020, 25, 705.	1.7	5
115	Non-equilibrium Quantum Brain Dynamics II: Formulation in 3+1 dimensions. Physica A: Statistical Mechanics and Its Applications, 2021, 567, 125706.	1.2	5
116	Computational prediction of heteromeric protein complex disassembly order using hybrid Monte Carlo/molecular dynamics simulation. Physical Chemistry Chemical Physics, 2022, 24, 10575-10587.	1.3	5
117	Triplet correlations and bridge functions in classical density functional theory for liquid water. Chemical Physics Letters, 2013, 572, 38-43.	1.2	4
118	Hierarchical coarse-graining model for photosystem II including electron and excitation-energy transfer processes. BioSystems, 2014, 117, 15-29.	0.9	4
119	Diffusion Monte Carlo study on temporal evolution of entropy and free energy in nonequilibrium processes. Journal of Chemical Physics, 2016, 144, 094103.	1.2	4
120	Four-electron model for singlet and triplet excitation energy transfers with inclusion of coherence memory, inelastic tunneling and nuclear quantum effects. Chemical Physics, 2016, 474, 18-24.	0.9	4
121	Machine learning prediction of inter-fragment interaction energies between ligand and amino-acid residues on the fragment molecular orbital calculations for Janus kinase â€“ inhibitor complex. Chemical Physics Letters, 2020, 757, 137883.	1.2	4
122	Remarked suppression of AÎ²₄₂ protomerâ€“protomer dissociation reaction elucidated by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1367-1375.	1.5	4
123	Derivation of extremely slow dynamics of protein motion based on entropy invariance. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 1280-1282.	0.9	3
124	Excitation energy transfer modulated by oscillating electronic coupling of a dimeric system embedded in a molecular environment. Physical Review E, 2012, 86, 021914.	0.8	3
125	Non-Equilibrium Quantum Brain Dynamics: Super-Radiance and Equilibration in 21 Dimensions+. Entropy, 2019, 21, 1066.	1.1	3
126	Appearance of Thermal Time. Foundations of Physics, 2021, 51, .	0.6	3

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127	Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules. , 2009, , 133-170.		3
128	Non-Equilibrium Quantum Electrodynamics in Open Systems as a Realizable Representation of Quantum Field Theory of the Brain. Entropy, 2020, 22, 43.	1.1	3
129	Elucidating microscopic events driven by GTP hydrolysis reaction in the Rasâ€“GAP system with semi-reactive molecular dynamics simulations: the alternative role of a phosphate binding loop for mechanical energy storage. Physical Chemistry Chemical Physics, 2021, 23, 26151-26164.	1.3	3
130	Quantum Brain Dynamics and Holography. Dynamics, 2022, 2, 187-218.	0.5	3
131	Renormalization-Group Inspired Approach to Vibrational Energy Transfer in Protein. Journal of the Physical Society of Japan, 2012, 81, 033801.	0.7	2
132	Variational Quantum Monte Carlo with Inclusion of Orbital Correlations. Journal of the Physical Society of Japan, 2013, 82, 075001.	0.7	2
133	Information geometrical characterization of the Onsager-Machlup process. Chemical Physics Letters, 2017, 689, 152-155.	1.2	2
134	Nonequilibrium quantum brain dynamics. Advances in Quantum Chemistry, 2020, 82, 159-180.	0.4	2
135	Nanoscale Quantum Thermal Conductance at Water Interface: Greenâ€™s Function Approach Based on One-Dimensional Phonon Model. Molecules, 2020, 25, 1185.	1.7	2
136	Temperature relaxation in binary hard-sphere mixture system: Molecular dynamics and kinetic theory study. Journal of Chemical Physics, 2020, 153, 034114.	1.2	1
137	Fragment Molecular Orbital Method as Cluster Expansion. , 2021, , 3-14.		1
138	FMO Drug Design Consortium. , 2021, , 127-181.		1
139	Improvement of the Force Field for Î²-d-Glucose with Machine Learning. Molecules, 2021, 26, 6691.	1.7	1
140	1P-100 Study of RNA base recognition mechanism by aliphatic surface of RNA-binding protein : Case study of NOVA-RNA complex system(Nucleic acid:Interaction & Complex formation, The 47th Annual) Tj ETQq0 0 0 rgBT /Overlock 10 Tf		0
141	Effects of Bridge Functions on Radial Distribution Functions of Liquid Water. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 152-156.	2.2	0
142	Comparison of Various Fragmentation Methods for Quantum Chemical Calculations of Large Molecular Systems. , 2021, , 15-27.		0
143	In silico modeling of PAX8â€“PPARÎ³ fusion protein in thyroid carcinoma: influence of structural perturbation by fusion on ligand-binding affinity. Journal of Computer-Aided Molecular Design, 2021, 35, 629-642.	1.3	0
144	Density-Matrix Based Scheme of Basis Selection for Linear Combination of Fragment Molecular Orbitals. Journal of the Physical Society of Japan, 2021, 90, 064301.	0.7	0

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145	1TP5-05 Study of RNA base recognition mechanism by aliphatic surface of RNA-binding protein : Case study of NOVA-RNA complex system(The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S37-S38.	0.0	0
146	Effects of bridge functions on radial distribution functions of liquid water. Interdisciplinary Sciences, Computational Life Sciences, 2014, , .	2.2	0
147	Quantum Brain Dynamics in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1106" altimg="si4.svg"><mml:mrow><mml:mn>2</mml:mn><mml:mo linebreak="goodbreak" linebreakstyle="after">+</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math> dimensions: Non-equilibrium analysis towards memory formations. Physica A: Statistical Mechanics and Its Applications, 2022, 598, 127397.	1.2	0