Yasuteru Shigeta

List of Publications by Year
in descending order

321 papers	5,440 citations	136740 32 h-index	123241 61 g-index
328 all docs	328 docs citations	328 times ranked	5427 citing authors

#	Article	IF	Citations
1	Phosphorylation in the accessory domain of yeast histone chaperone protein 1 exposes the nuclear export signal sequence. Proteins: Structure, Function and Bioinformatics, 2022, 90, 317-321.	1.5	2
2	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. Journal of Computational Chemistry, 2022, 43, 206-214.	1.5	4
3	Ligand Binding Path Sampling Based on Parallel Cascade Selection Molecular Dynamics: LB-PaCS-MD. Materials, 2022, 15, 1490.	1.3	1
4	The role of <scp>ATP</scp> in solubilizing <scp>RNA</scp>â€binding protein fused in sarcoma. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1606-1612.	1.5	11
5	Halogenated Baicalein as a Promising Antiviral Agent toward SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2022, 62, 1498-1509.	2.5	30
6	Semi-Synthesis of N-Aryl Amide Analogs of Piperine from Piper nigrum and Evaluation of Their Antitrypanosomal, Antimalarial, and Anti-SARS-CoV-2 Main Protease Activities. Molecules, 2022, 27, 2841.	1.7	10
7	Evaluation of an Appropriate Standard Hydrogen Electrode Potential for Computing Redox Potentials of Catechins with Density Functional Theory. Chemistry Letters, 2022, 51, 673-677.	0.7	0
8	Heme-bound tyrosine vibrations in hemoglobin M: Resonance Raman, crystallography, and DFT calculation. Biophysical Journal, 2022, 121, 2767-2780.	0.2	3
9	Structural Validation by the G-Factor Properly Regulates Boost Potentials Imposed in Conformational Sampling of Proteins. Journal of Chemical Information and Modeling, 2022, 62, 3442-3452.	2.5	2
10	Conformation-Changeable Ï€-Electronic Systems with Metastable Bent-Core Conformations and Liquid-Crystalline-State Electric-Field-Responsive Properties. Organic Letters, 2021, 23, 305-310.	2.4	4
11	Ion-pairing Ï€-electronic systems: ordered arrangement and noncovalent interactions of negatively charged porphyrins. Chemical Science, 2021, 12, 9645-9657.	3.7	23
12	In silico mutational analyses reveal different ligand-binding abilities of double pockets of medaka fish taste receptor type 1 essential for efficient taste recognition. Physical Chemistry Chemical Physics, 2021, 23, 20398-20405.	1.3	0
13	Interaction of 8-anilinonaphthalene-1-sulfonate with SARS-CoV-2 main protease and its application as a fluorescent probe for inhibitor identification. Computational and Structural Biotechnology Journal, 2021, 19, 3364-3371.	1.9	26
14	Molecular Motions of Imidazole in Poly(vinylphosphonic acid)-Imidazole Composites Investigated by Molecular Dynamics Simulations. Chemistry Letters, 2021, 50, 17-20.	0.7	4
15	AnalysisFMO Toolkit: A PyMOL Plugin for 3D-Visualization of Interaction Energies in Proteins (3D-VIEP) Calculated by the FMO Method. , 2021, , 357-370.		0
16	The Folding of Trp-cage is Regulated by Stochastic Flip of the Side Chain of Tryptophan. Chemistry Letters, 2021, 50, 162-165.	0.7	3
17	Estimation of the relative contributions to the electronic energy transfer rates based on FÃ¶rster theory: The case of C-phycocyanin chromophores. Biophysics and Physicobiology, 2021, 18, 196-214.	0.5	3
18	Linear Combination of Molecular Orbitals of Fragments (FMO-LCMO) Method: Its Application to Charge Transfer Studies. , 2021, , 391-405.		1

#	Article	IF	Citations
19	Computational Analysis Reveals a Critical Point Mutation in the N-Terminal Region of the Signaling Lymphocytic Activation Molecule Responsible for the Cross-Species Infection with Canine Distemper Virus. Molecules, 2021, 26, 1262.	1.7	4
20	Split conformation of Chaetomium thermophilum Hsp104 disaggregase. Structure, 2021, 29, 721-730.e6.	1.6	2
21	Comparison between the Light-Harvesting Mechanisms of Type-I Photosynthetic Reaction Centers of Heliobacteria and Photosystem I: Pigment Site Energy Distribution and Exciton State. Journal of Physical Chemistry B, 2021, 125, 3727-3738.	1.2	5
22	Weak O2 binding and strong H2O2 binding at the non-heme diiron center of trypanosome alternative oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148356.	0.5	7
23	Structure, solubility, and permeability relationships in a diverse middle molecule library. Bioorganic and Medicinal Chemistry Letters, 2021, 37, 127847.	1.0	3
24	Proton Conduction Mechanism for Anhydrous Imidazolium Hydrogen Succinate Based on Local Structures and Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 5390-5394.	2.1	18
25	pyProGAâ€"A PyMOL plugin for protein residue network analysis. PLoS ONE, 2021, 16, e0255167.	1.1	10
26	On-Demand Chirality Transfer of Human Serum Albumin to Bis(thiophen-2-yl)hexafluorocyclopentenes through Their Photochromic Ring Closure. Journal of Organic Chemistry, 2021, 86, 12549-12558.	1.7	8
27	A Practical Prediction of LogPo/w through Semiempirical Electronic Structure Calculations with Dielectric Continuum Model. Bulletin of the Chemical Society of Japan, 2021, 94, 1807-1814.	2.0	3
28	Could London Dispersion Force Control Regioselective (2 + 2) Cyclodimerizations of Benzynes? YES: Application to the Synthesis of Helical Biphenylenes. Journal of the American Chemical Society, 2021, 143, 10853-10859.	6.6	19
29	Control of chirality, bond flexing and anharmonicity in an electric field. International Journal of Quantum Chemistry, 2021, 121, e26793.	1.0	8
30	Solvophobicity-directed assembly of microporous molecular crystals. Communications Chemistry, 2021, 4, .	2.0	7
31	Independent Nontargeted Parallel Cascade Selection Molecular Dynamics (Ino-PaCS-MD) to Enhance the Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2021, 17, 5933-5943.	2.3	2
32	Chirality without Stereoisomers: Insight fromÂthe Helical Response of Bond Electrons. ChemPhysChem, 2021, 22, 1989-1995.	1.0	8
33	Solubility and Membrane Permeability of Cyclic Dipeptides Approximately Estimated by Quantum Chemistry and Molecular Dynamics Calculations. Chemistry Letters, 2021, 50, 1964-1967.	0.7	1
34	A post-process to estimate an approximated minimal free energy path based on local centroids. Chemical Physics Letters, 2021, 782, 139003.	1.2	2
35	Rearrangements of Water Molecules in Parallel Cascade Selection Molecular Dynamics Enhance Structural Explorations of Proteins. Bulletin of the Chemical Society of Japan, 2021, 94, 97-105.	2.0	1
36	Structural and functional characterization of nylon hydrolases. Methods in Enzymology, 2021, 648, 357-389.	0.4	8

#	Article	IF	Citations
37	Effects of mechanical grinding on the phase behavior and anhydrous proton conductivity of imidazolium hydrogen succinate. Solid State Ionics, 2021, 372, 115775.	1.3	4
38	Structural Variations of Metallothionein with or without Zinc Ions Elucidated by All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 12712-12717.	1.2	1
39	Alkyne-Tagged Apigenin, a Chemical Tool to Navigate Potential Targets of Flavonoid Anti-Dengue Leads. Molecules, 2021, 26, 6967.	1.7	4
40	A Free-Energy Landscape Analysis of Calmodulin Obtained from an NMR Data-Utilized Multi-Scale Divide-and-Conquer Molecular Dynamics Simulation. Life, 2021, 11, 1241.	1.1	0
41	Residue Folding Degreeâ€"Relationship to Secondary Structure Categories and Use as Collective Variable. International Journal of Molecular Sciences, 2021, 22, 13042.	1.8	3
42	Experimental and theoretical study on converting myoglobin into a stable domain-swapped dimer by utilizing a tight hydrogen bond network at the hinge region. RSC Advances, 2021, 11, 37604-37611.	1.7	2
43	Theoretical Prediction of the Redox Potential of Catechins with First Principle Calculation. Journal of Computer Chemistry Japan, 2021, 20, 137-139.	0.0	0
44	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. J, 2021, 4, 849-864.	0.6	7
45	Multiple Virtual Screening Strategies for the Discovery of Novel Compounds Active Against Dengue Virus: A Hit Identification Study. Scientia Pharmaceutica, 2020, 88, 2.	0.7	24
46	Reaction of threonine synthase with the substrate analogue 2-amino-5-phosphonopentanoate: implications into the proton transfer at the active site. Journal of Biochemistry, 2020, 167, 357-364.	0.9	0
47	Tunneling matrix element and tunneling pathways of protein electron transfer calculated with a fragment molecular orbital method. Journal of Chemical Physics, 2020, 153, 104104.	1.2	2
48	Efficient Conformational Sampling of Collective Motions of Proteins with Principal Component Analysis-Based Parallel Cascade Selection Molecular Dynamics. Journal of Chemical Information and Modeling, 2020, 60, 4021-4029.	2.5	10
49	Self-Associating Curved Ï€-Electronic Systems with Electron-Donating and Hydrogen-Bonding Properties. Journal of the American Chemical Society, 2020, 142, 16420-16428.	6.6	12
50	Enhanced Conformational Sampling Method Based on Anomaly Detection Parallel Cascade Selection Molecular Dynamics: ad-PaCS-MD. Journal of Chemical Theory and Computation, 2020, 16, 6716-6725.	2.3	2
51	Dibromopinocembrin and Dibromopinostrobin Are Potential Anti-Dengue Leads with Mild Animal Toxicity. Molecules, 2020, 25, 4154.	1.7	16
52	Molecular Mechanism for the Actin-Binding Domain of Î±-Actinin Ain1 Elucidated by Molecular Dynamics Simulations and Mutagenesis Experiments. Journal of Physical Chemistry B, 2020, 124, 8495-8503.	1.2	3
53	Regenerations of Initial Velocities in Parallel Cascade Selection Molecular Dynamics (PaCS-MD) Enhance the Conformational Transitions of Proteins. Chemistry Letters, 2020, 49, 798-801.	0.7	5
54	Understanding the Detection Mechanisms and Ability of Molecular Hydrogen on Three-Dimensional Bicontinuous Nanoporous Reduced Graphene Oxide. Materials, 2020, 13, 2259.	1.3	0

#	Article	IF	Citations
55	Neutron crystallography of copper amine oxidase reveals keto/enolate interconversion of the quinone cofactor and unusual proton sharing. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10818-10824.	3.3	11
56	Analytical Method Using a Scaled Hypersphere Search for High-Dimensional Metadynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 3869-3878.	2.3	7
57	Distribution of Counter Ions in Negatively-charged Lipid/Water/Air Interface: Molecular Dynamics Study. Chemistry Letters, 2020, 49, 361-363.	0.7	1
58	The Dynamics of S-adenosyl-methionine and S-adenosyl-homocysteine in Mouse Dnmt1 is Driven by Their Structural Flexibilities. Chemistry Letters, 2020, 49, 785-788.	0.7	1
59	Protein Dynamics and the Folding Degree. Journal of Chemical Information and Modeling, 2020, 60, 1559-1567.	2.5	5
60	Local Structures and Dynamics of Imidazole Molecules in Poly(vinylphosphonic acid)â€“Imidazole Composite Investigated by Molecular Dynamics. ACS Applied Polymer Materials, 2020, 2, 1561-1568.	2.0	11
61	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. Physical Chemistry Chemical Physics, 2020, 22, 2509-2520.	1.3	19
62	Excitonic Coupling on a Heliobacterial Symmetrical Type-I Reaction Center: Comparison with Photosystem I. Journal of Physical Chemistry B, 2020, 124, 389-403.	1.2	8
63	Target Identification Using Homopharma and Network-Based Methods for Predicting Compounds Against Dengue Virus-Infected Cells. Molecules, 2020, 25, 1883.	1.7	4
64	Why Are Lopinavir and Ritonavir Effective against the Newly Emerged Coronavirus 2019? Atomistic Insights into the Inhibitory Mechanisms. Biochemistry, 2020, 59, 1769-1779.	1.2	187
65	Estimation of Acid Dissociation Constants (pK_a) of N-Containing Heterocycles in DMSO and Transferability of Gibbs Free Energy in Different Solvent Conditions. Chemistry Letters, 2020, 49, 307-310.	0.7	5
66	Agonist and Antagonist-Diverted Twisting Motions of a Single TRPV1 Channel. Journal of Physical Chemistry B, 2020, 124, 11617-11624.	1.2	13
67	Reaction mechanism of N-cyclopropylglycine oxidation by monomeric sarcosine oxidase. Physical Chemistry Chemical Physics, 2020, 22, 16552-16561.	1.3	4
68	Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase. RSC Advances, 2020, 10, 38631-38639.	1.7	8
69	Role of the Propionic Acid Side-Chain of C-Phycocyanin Chromophores in the Excited States for the Photosynthesis Process. Bulletin of the Chemical Society of Japan, 2020, 93, 1509-1519.	2.0	8
70	Photosynergetic Effects on Tripletâ€“Triplet Annihilation Upconversion Processes in Solid Studied by Theory and Experiments. , 2020, , 147-170.		0
71	Numerical investigation of the nano-scale solutal Marangoni convections. Journal of the Taiwan Institute of Chemical Engineers, 2019, 98, 20-26.	2.7	6
72	Parallel Cascade Selection Molecular Dynamics Simulations for Transition Pathway Sampling of Biomolecules. Advances in Quantum Chemistry, 2019, , 129-147.	0.4	0

#	Article	IF	Citations
73	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Waterâ€“Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.	2.1	43
74	Parallel cascade selection molecular dynamics to screen for protein complexes generated by rigid docking. Journal of Molecular Graphics and Modelling, 2019, 92, 94-99.	1.3	1
75	Nontargeted Parallel Cascade Selection Molecular Dynamics Based on a Nonredundant Selection Rule for Initial Structures Enhances Conformational Sampling of Proteins. Journal of Chemical Information and Modeling, 2019, 59, 5198-5206.	2.5	5
76	Selection Rules for Outliers in Outlier Flooding Method Regulate Its Conformational Sampling Efficiency. Journal of Chemical Information and Modeling, 2019, 59, 3919-3926.	2.5	2
77	Nontargeted Parallel Cascade Selection Molecular Dynamics Using Time-Localized Prediction of Conformational Transitions in Protein Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 5144-5153.	2.3	12
78	Possible Configurations of Apo-form Taste Receptor Type 1 (T1r) Studied by Microsecond-order Molecular Dynamics Simulation. Chemistry Letters, 2019, 48, 325-328.	0.7	1
79	Structural Changes of the Trinuclear Copper Center in Bilirubin Oxidase upon Reduction. Molecules, 2019, 24, 76.	1.7	3
80	Quadruply N-methylated octaphyrin: a helical macrocycle exhibiting chiroptical properties and dynamic conformation changes correlated with helical and inner N-methyl orientations. Organic and Biomolecular Chemistry, 2019, 17, 1163-1168.	1.5	8
81	First-Principles Study of the Reaction Mechanism of CHO + H on Graphene Surface. Journal of Physical Chemistry A, 2019, 123, 5633-5639.	1.1	3
82	Elucidation of the entire Kok cycle for photosynthetic water oxidation by the large-scale quantum mechanics/molecular mechanics calculations: Comparison with the experimental results by the recent serial femtosecond crystallography. Chemical Physics Letters, 2019, 730, 416-425.	1.2	8
83	Pyrroleâ€Based Ïâ€Systemâ€“Pt^{II} Complexes: Chiroptical Properties and Excitedâ€State Dynamics with Microsecond Triplet Lifetimes. Chemistry - A European Journal, 2019, 25, 8797-8804.	1.7	6
84	In Silico Structural Modeling and Analysis of Elongation Factor-1 Alpha and Elongation Factor-like Protein. ACS Omega, 2019, 4, 7308-7316.	1.6	5
85	Temperatureâ€“pressure shuffling outlier flooding method enhances the conformational sampling of proteins. Journal of Computational Chemistry, 2019, 40, 1530-1537.	1.5	4
86	Chiralityâ€“Helicity Equivalence in the S and R Stereoisomers: AÂTheoretical Insight. Journal of the American Chemical Society, 2019, 141, 5497-5503.	6.6	29
87	Photosubstitution Reaction of cis-[Ru(bpy)₂(CH₃CN)₂]²⁺ and cis-[Ru(bpy)₂(NH₃)₂]²⁺ in Aqueous Solution via Monoaqua Intermediate. Journal of Physical Chemistry A, 2019, 123, 2497-2502.	1.1	8
88	Reaction mechanism of non-enzymatic stereoselective formation of wine lactone. Chemical Physics Letters, 2019, 725, 114-118.	1.2	0
89	Effects of Antifreezing Protein from Rhagium inquisitor Binding on Ice Growth: A Molecular Dynamics Study. Chemistry Letters, 2019, 48, 223-226.	0.7	0
90	The Study of the Octanol-Water Partition Coefficient by the Computational Chemistry Method. Journal of Computer Chemistry Japan, 2019, 18, 241-243.	0.0	1

#	Article	IF	Citations
91	New assay method based on Raman spectroscopy for enzymes reacting with gaseous substrates. Protein Science, 2019, 28, 663-670.	3.1	5
92	Hybrid Cascade-Type Molecular Dynamics with a Markov State Model for Efficient Free Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 680-687.	2.3	12
93	Theoretical study of the photodissociation reaction of methanol. Chemical Physics Letters, 2019, 714, 137-142.	1.2	8
94	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.	2.5	13
95	First-principle study of ammonia decomposition and nitrogen incorporation on the GaN surface in metal organic vapor phase epitaxy. Journal of Crystal Growth, 2019, 507, 421-424.	0.7	6
96	Calculation of Free Energy Reaction Network of Alanine Polypeptide by Using Free Energy Reaction Route Mapping Method. Journal of Computer Chemistry Japan, 2019, 18, 221-223.	0.0	0
97	Developments of Rare Event Sampling Methods for Proteins. Journal of Computer Chemistry Japan, 2019, 18, 199-201.	0.0	0
98	Does Inactive Alkyl Chain Enhance Tripletâ€“Triplet Annihilation of 9,10-Diphenylanthracene Derivatives?. Journal of Physical Chemistry C, 2018, 122, 5334-5340.	1.5	14
99	The effect of octahedral distortions on the electronic properties and magnetic interactions in O3 NaTMO₂ compounds (TM = Tiâ€“Ni & Zrâ€“Pd). RSC Advances, 2018, 8, 13842-13849.	1.7	18
100	Dominant role of orbital splitting in determining cathode potential in O3 NaTMO2 compounds. Journal of Power Sources, 2018, 388, 1-4.	4.0	12
101	Programed dynamical ordering in self-organization processes of a nanocube: a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 9115-9122.	1.3	7
102	First-principles study of the formation of glycine-producing radicals from common interstellar species. Molecular Astrophysics, 2018, 10, 11-19.	1.7	22
103	The binding structure and affinity of photodamaged duplex DNA with members of the photolyase/cryptochrome family: A computational study. Biophysics and Physicobiology, 2018, 15, 18-27.	0.5	7
104	Nonadiabatic one-electron transfer mechanism for the Oâ€“O bond formation in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2018, 698, 138-146.	1.2	28
105	Molecular association model of PPARÎ± and its new specific and efficient ligand, pemafibrate: Structural basis for SPPARMÎ±. Biochemical and Biophysical Research Communications, 2018, 499, 239-245.	1.0	47
106	An assessment of optimal time scale of conformational resampling for parallel cascade selection molecular dynamics. Molecular Simulation, 2018, 44, 206-212.	0.9	6
107	The Formation of Hydrophobic Core Regulates the Protein Folding of Villin Elucidated with Parallel Cascade Selection Molecular Dynamics. Chemistry Letters, 2018, 47, 1300-1303.	0.7	0
108	Protein Residue Networks from Energetic and Geometric Data: Are They Identical?. Journal of Chemical Theory and Computation, 2018, 14, 6623-6631.	2.3	24

#	Article	IF	Citations
109	A Theoretical Study on Redox Potential and pKa of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	2.0	4
110	Reaction Pathway of Surface-Catalyzed Ammonia Decomposition and Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride. Journal of Physical Chemistry C, 2018, 122, 24665-24671.	1.5	10
111	Synergetic Effects of Tripletâ€“Triplet Annihilation and Directional Triplet Exciton Migration in Organic Crystals for Photon Upconversion. Journal of Physical Chemistry Letters, 2018, 9, 6638-6643.	2.1	23
112	Selection rules on initial structures in parallel cascade selection molecular dynamics affect conformational sampling efficiency. Journal of Molecular Graphics and Modelling, 2018, 85, 153-159.	1.3	3
113	High-performance Na ion cathodes based on the ubiquitous and reversible O redox reaction. Journal of Materials Chemistry A, 2018, 6, 24120-24127.	5.2	5
114	Redox Potentialâ€Đependent Formation of an Unusual Hisâ€“Trp Bond in Bilirubin Oxidase. Chemistry - A European Journal, 2018, 24, 18052-18058.	1.7	14
115	Coulomb and CHâ€“Ï€Âinteractions in (6â€“4) photolyaseâ€“DNA complex dominate DNA binding and repair abilities. Nucleic Acids Research, 2018, 46, 6761-6772.	6.5	11
116	Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in PhotosystemÂII. Journal of Physical Chemistry B, 2018, 122, 6491-6502.	1.2	21
117	On-the-Fly Specifications of Reaction Coordinates in Parallel Cascade Selection Molecular Dynamics Accelerate Conformational Transitions of Proteins. Journal of Chemical Theory and Computation, 2018, 14, 3332-3341.	2.3	9
118	Novel Techniques for Observing Structural Dynamics of Photoresponsive Liquid Crystals. Journal of Visualized Experiments, 2018, , .	0.2	2
119	A Practical Approach for Searching Stable Molecular Structures by Introducing Repulsive Interactions among Walkers. Bulletin of the Chemical Society of Japan, 2018, 91, 1465-1473.	2.0	4
120	A computational scheme of pK_a values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. Physical Chemistry Chemical Physics, 2018, 20, 27272-27279.	1.3	11
121	Computational electrochemistry of a novel ferrocene derivative. Journal of Molecular Graphics and Modelling, 2018, 85, 84-90.	1.3	2
122	How Does Friction Coefficient Affect the Conformational Sampling Efficiency of Parallel Cascade Selection Molecular Dynamics?. Chemistry Letters, 2018, 47, 1119-1122.	0.7	1
123	How low-resolution structural data predict the conformational changes of a protein: a study on data-driven molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 17790-17798.	1.3	3
124	Temperature-Shuffled Structural Dissimilarity Sampling Based on a Root-Mean-Square Deviation. Journal of Chemical Information and Modeling, 2018, 58, 1397-1405.	2.5	9
125	Analyses on Dynamical Ordering of Protein Functions by Means of Cascade Selection Molecular Dynamics. Journal of Computer Chemistry Japan, 2018, 17, 46-56.	0.0	0
126	Molecular Dynamics studies on the effects of Antifreezing Protein from Rhagium inquisitor (RiAFP) on Ice Growth. Journal of Computer Chemistry Japan, 2018, 17, 222-224.	0.0	0

#	Article	IF	Citations
127	The Reaction Mechanisms of O₂ Formation in Photosynthesis. Seibutsu Butsuri, 2018, 58, 127-133.	0.0	0
128	Cooperatively Interlocked [2+1]â€Type Ï€â€Systemâ€“Anion Complexes. Chemistry - A European Journal, 2017, 23, 4160-4168.	1.7	17
129	Outstanding Reviewers for Physical Chemistry Chemical Physics in 2016. Physical Chemistry Chemical Physics, 2017, 19, 8140-8140.	1.3	0
130	Efficient Conformational Search Based on Structural Dissimilarity Sampling: Applications for Reproducing Structural Transitions of Proteins. Journal of Chemical Theory and Computation, 2017, 13, 1411-1423.	2.3	26
131	Common folding processes of mini-proteins: Partial formations of secondary structures initiate the immediate protein folding. Journal of Computational Chemistry, 2017, 38, 790-797.	1.5	10
132	Molecular Mechanism of the Reaction Specificity in Threonine Synthase: Importance of the Substrate Conformations. Journal of Physical Chemistry B, 2017, 121, 5536-5543.	1.2	3
133	Identification of the key interactions in structural transition pathway of FtsZ from Staphylococcus aureus. Journal of Structural Biology, 2017, 198, 65-73.	1.3	41
134	Direct Observation of the Ultrafast Evolution of Open-Shell Biradical in Photochromic Radical Dimer. Journal of the American Chemical Society, 2017, 139, 6382-6389.	6.6	23
135	Structural dissimilarity sampling with dynamically self-guiding selection. Journal of Computational Chemistry, 2017, 38, 1921-1929.	1.5	11
136	Theoretical Analyses of Tripletâ€“Triplet Annihilation Process of 9,10-Diphenylanthracene in Solution. Chemistry Letters, 2017, 46, 873-875.	0.7	11
137	How Does the Number of Initial Structures Affect the Conformational Sampling Efficiency and Quality in Parallel Cascade Selection Molecular Dynamics (PaCS-MD)?. Chemistry Letters, 2017, 46, 862-865.	0.7	8
138	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. Polyhedron, 2017, 136, 125-131.	1.0	8
139	Large-scale QM/MM calculations of the CaMn₄O₅ cluster in the S₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. Faraday Discussions, 2017, 198, 83-106.	1.6	31
140	H-Aggregated Ï€-Systems Based on Disulfide-Linked Dimers of Dipyrrolyldiketone Boron Complexes. Journal of Organic Chemistry, 2017, 82, 11166-11172.	1.7	7
141	A theoretical study of the formation of glycine via hydantoin intermediate in outer space environment. Chemical Physics Letters, 2017, 687, 178-183.	1.2	22
142	Structural Monitoring of the Onset of Excited-State Aromaticity in a Liquid Crystal Phase. Journal of the American Chemical Society, 2017, 139, 15792-15800.	6.6	59
143	Classical cumulant dynamics for statistical chemical physics. Molecular Simulation, 2017, 43, 1260-1268.	0.9	0
144	Mechanistic Insight into Weak Baseâ€Catalyzed Generation of Carbon Monoxide from Phenyl Formate and Its Application to Catalytic Carbonylation at Room Temperature without Use of External Carbon Monoxide Gas. Advanced Synthesis and Catalysis, 2017, 359, 3592-3601.	2.1	19

#	Article	IF	Citations
145	Dynamic Specification of Initial Structures in Parallel Cascade Selection Molecular Dynamics (PaCS-MD) Efficiently Promotes Biologically Relevant Rare Events. Bulletin of the Chemical Society of Japan, 2017, 90, 1236-1243.	2.0	8
146	Temperatureâ€shuffled parallel cascade selection molecular dynamics accelerates the structural transitions of proteins. Journal of Computational Chemistry, 2017, 38, 2671-2674.	1.5	23
147	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK_a for Several Chemical Groups. Journal of Chemical Theory and Computation, 2017, 13, 4791-4803.	2.3	25
148	Phototransformative Supramolecular Assembly of Amphiphilic Diarylethenes Realized by a Combination of Photochromism and Lower Critical Solution Temperature Behavior. Chemistry - A European Journal, 2017, 23, 15059-15066.	1.7	15
149	Self-Avoiding Conformational Sampling Based on Histories of Past Conformational Searches. Journal of Chemical Information and Modeling, 2017, 57, 3070-3078.	2.5	7
150	Integrated Computational Studies on Mutational Effects of a Nylon-Degrading Enzyme. Progress in Theoretical Chemistry and Physics, 2017, , 317-330.	0.2	0
151	TaBoo SeArch Algorithm with a Modified Inverse Histogram for Reproducing Biologically Relevant Rare Events of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 2436-2445.	2.3	9
152	Refractive indices of organoâ€metallic and â€metalloid compounds: A longâ€range corrected DFT study. Journal of Computational Chemistry, 2016, 37, 2759-2769.	1.5	4
153	Mutations affecting the internal equilibrium of the reaction catalyzed by 6â€aminohexanoateâ€dimer hydrolase. FEBS Letters, 2016, 590, 3133-3143.	1.3	1
154	Ion-Pairing Crystal Polymorphs of Interlocked [2 + 1]-Type Receptorâ€“Anion Complexes. Journal of Organic Chemistry, 2016, 81, 8530-8536.	1.7	9
155	A Fast Convergent Simulated Annealing Algorithm for Protein-Folding: Simulated Annealing Outlier FLOODing (SA-OFLOOD) Method. Bulletin of the Chemical Society of Japan, 2016, 89, 1361-1367.	2.0	19
156	Theoretical analyses on a flipping mechanism of UV-induced DNA damage. Biophysics and Physicobiology, 2016, 13, 311-319.	0.5	8
157	Molecular mechanisms of substrate specificities of uridine-cytidine kinase. Biophysics and Physicobiology, 2016, 13, 77-84.	0.5	6
158	Doubly N-Methylated Porphyrinoids. Organic Letters, 2016, 18, 3006-3009.	2.4	8
159	Sparsityâ€weighted outlier <scp>FLOOD</scp>ing (<scp>OFLOOD</scp>) method: Efficient rare event sampling method using sparsity of distribution. Journal of Computational Chemistry, 2016, 37, 724-738.	1.5	20
160	Catalytic Mechanism of Nitrile Hydratase Subsequent to Cyclic Intermediate Formation: A QM/MM Study. Journal of Physical Chemistry B, 2016, 120, 3259-3266.	1.2	14
161	Solvent effects on excited-state electron-transfer rate of pyrene-labeled deoxyuridine: A theoretical study. Chemical Physics Letters, 2016, 644, 25-30.	1.2	5
162	Ultrafast Snapshots of the Molecules Twisting in Liquid Crystal State. , 2016, , .		0

#	Article	IF	Citations
163	Automatic detection of hidden dimensions to obtain appropriate reaction coordinates in the Outlier FLOODing (OFLOOD) method. Chemical Physics Letters, 2015, 639, 269-274.	1.2	17
164	Approximate spin projected spin-unrestricted density functional theory method: Application to diradical character dependences of second hyperpolarizabilities. , 2015, , .		1
165	Ab initio molecular orbital-configuration interaction based quantum master equation (MOQME) approach to the dynamic first hyperpolarizabilities of asymmetric Ï€-conjugated systems. , 2015, , .		0
166	Relationship between second hyperpolarizability and diradical character in open-shell singlet metalâ€“metal multiply bonded systems. , 2015, , .		0
167	Simple, yet powerful methodologies for conformational sampling of proteins. Physical Chemistry Chemical Physics, 2015, 17, 6155-6173.	1.3	55
168	Efficient conformational sampling of proteins based on a multi-dimensional TaBoo SeArch algorithm: An application to folding of chignolin in explicit solvent. Chemical Physics Letters, 2015, 630, 68-75.	1.2	9
169	A QM/MM study of the initial steps of catalytic mechanism of nitrile hydratase. Chemical Physics Letters, 2015, 623, 8-13.	1.2	8
170	Accurate Standard Hydrogen Electrode Potential and Applications to the Redox Potentials of Vitamin C and NAD/NADH. Journal of Physical Chemistry A, 2015, 119, 369-376.	1.1	102
171	Protein folding pathways extracted by OFLOOD: Outlier FLOODing method. Journal of Computational Chemistry, 2015, 36, 97-102.	1.5	30
172	Theoretical design of solvatochromism switching by photochromic reactions using donorâ€“acceptor disubstituted diarylethene derivatives with oxidized thiophene rings. Physical Chemistry Chemical Physics, 2015, 17, 6484-6494.	1.3	4
173	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.	0.8	6
174	Enhanced conformational sampling method for proteins based on the <scp>T</scp>a<scp>B</scp>oo <scp>S</scp>e<scp>A</scp>rch algorithm: Application to the folding of a miniâ€protein, chignolin. Journal of Computational Chemistry, 2015, 36, 763-772.	1.5	20
175	Theoretical Study on Reaction Mechanisms of Nitrite Reduction by Copper Nitrite Complexes: Toward Understanding and Controlling Possible Mechanisms of Copper Nitrite Reductase. Journal of Physical Chemistry B, 2015, 119, 5392-5403.	1.2	14
176	Unraveling the degradation of artificial amide bonds in nylon oligomer hydrolase: from induced-fit to acylation processes. Physical Chemistry Chemical Physics, 2015, 17, 4492-4504.	1.3	12
177	Performance of the divide-and-conquer approach used as an initial guess. Chemical Physics Letters, 2015, 634, 181-187.	1.2	3
178	Quantal cumulant dynamics for realâ€time simulations of quantum manyâ€body systems. International Journal of Quantum Chemistry, 2015, 115, 300-308.	1.0	5
179	Substitution effects on optical properties of iminonitroxide- substituted iminonitroxide diradical. Molecular Physics, 2015, 113, 267-273.	0.8	1
180	Static electric field effect on third-order nonlinear optical (NLO) properties of singlet diradical molecules: Toward the realization of an electric field induced open-shell NLO switch. , 2015, , .		0

#	Article	IF	Citations
181	On the inducedâ€fit mechanism of substrateâ€enzyme binding structures of nylonâ€oligomer hydrolase. Journal of Computational Chemistry, 2014, 35, 1240-1247.	1.5	23
182	A density functional study on the pK_a of small polyprotic molecules. International Journal of Quantum Chemistry, 2014, 114, 1128-1134.	1.0	30
183	Fluctuation Flooding Method (FFM) for accelerating conformational transitions of proteins. Journal of Chemical Physics, 2014, 140, 125103.	1.2	25
184	Nylon-Oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds. Journal of Physical Chemistry Letters, 2014, 5, 1210-1216.	2.1	13
185	Open-Shell Character and Second Hyperpolarizabilities of One-Dimensional Chromium(II) Chains: Size Dependence and Bond-Length Alternation Effect. Inorganic Chemistry, 2014, 53, 8700-8707.	1.9	10
186	Comparative study of diradical characters and thirdâ€order nonlinear optical properties of linear/cyclic acenes versus phenylenes. International Journal of Quantum Chemistry, 2013, 113, 592-598.	1.0	15
187	Diradicalology in thirdâ€order nonlinear optical systems: Second hyperpolarizabilities of acetyleneâ€linked phenalenylâ€based superpolyenes. International Journal of Quantum Chemistry, 2013, 113, 585-591.	1.0	4
188	Quantal cumulant mechanics and dynamics for multidimensional quantum manyâ€body clusters. International Journal of Quantum Chemistry, 2013, 113, 348-355.	1.0	9
189	Antidot effects on the openâ€shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. International Journal of Quantum Chemistry, 2013, 113, 605-611.	1.0	3
190	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. Journal of Physical Chemistry Letters, 2013, 4, 2418-2422.	2.1	48
191	Binding of a Positron to Nucleic Base Molecules and Their Pairs. ChemPhysChem, 2013, 14, 3458-3462.	1.0	10
192	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional Nin (n = 3, 5, 7) complexes. Dalton Transactions, 2013, 42, 16200.	1.6	18
193	Synthesis and Characterization of Quarteranthene: Elucidating the Characteristics of the Edge State of Graphene Nanoribbons at the Molecular Level. Journal of the American Chemical Society, 2013, 135, 1430-1437.	6.6	237
194	Interplay between the Diradical Character and ThirdâEOrder Nonlinear Optical Properties in Fullerene Systems. Chemistry - A European Journal, 2013, 19, 1677-1685.	1.7	36
195	A new type of organicâ€“inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. Dalton Transactions, 2013, 42, 15053.	1.6	111
196	Non-empirical tuning of CAM-B3LYP functional in time-dependent density functional theory for excitation energies of diarylethene derivatives. Chemical Physics Letters, 2013, 585, 201-206.	1.2	31
197	A Density Functional Theory Based Protocol to Compute the Redox Potential of Transition Metal Complex with the Correction of Pseudo-Counterion: General Theory and Applications. Journal of Chemical Theory and Computation, 2013, 9, 2974-2980.	2.3	36
198	Finiteâ€field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an openâ€shell singlet molecule in solvents. Journal of Computational Chemistry, 2013, 34, 2345-2352.	1.5	1

#	Article	IF	Citations
199	Atom-Scale Reaction Pathways and Free-Energy Landscapes in Oxygen Plasma Etching of Graphene. Journal of Physical Chemistry Letters, 2013, 4, 1592-1596.	2.1	31
200	Consistent scheme for computing standard hydrogen electrode and redox potentials. Journal of Computational Chemistry, 2013, 34, 21-26.	1.5	39
201	I-V characteristics of several modified DNA bases. , 2012, , .		0
202	DFT Analysis of Low-frequency Heme Vibrations in Soluble Guanylate Cyclase: Raman Mode Enhancement by Propionateâ€“Protein Interactions. Chemistry Letters, 2012, 41, 860-862.	0.7	0
203	Temperature-Independent Stereoselectivity in Intramolecular Cycloaddition of Ketene Generated from Diazoester in Solution and in Vapor Phase: How Entropy Term Governs the Selectivity. Bulletin of the Chemical Society of Japan, 2012, 85, 504-510.	2.0	2
204	Development of Calculation and Analysis Methods for the Dynamic First Hyperpolarizability Based on the Ab Initio Molecular Orbital â€“ Quantum Master Equation Method. Journal of Physical Chemistry A, 2012, 116, 4371-4380.	1.1	4
205	Halide Ion Complexes of Decaborane (B₁₀H₁₄) and Their Derivatives: Noncovalent Charge Transfer Effect on Second-Order Nonlinear Optical Properties. Journal of Physical Chemistry A, 2012, 116, 1417-1424.	1.1	62
206	Computational study toward micro electronics engineering. , 2012, , .		0
207	Enhancement of the Third-Order Nonlinear Optical Properties in Open-Shell Singlet Transition-Metal Dinuclear Systems: Effects of the Group, of the Period, and of the Charge of the Metal Atom. Journal of Physical Chemistry A, 2012, 116, 5501-5509.	1.1	25
208	Theoretical Insight into Stereoselective Reaction Mechanisms of 2,4-Pentanediol-Tethered Ketene-Olefin [2 + 2] Cycloaddition. Journal of Physical Chemistry A, 2012, 116, 1168-1175.	1.1	7
209	Impact of Antidot Structure on the Multiradical Characters, Aromaticities, and Third-Order Nonlinear Optical Properties of Hexagonal Graphene Nanoflakes. Journal of Physical Chemistry C, 2012, 116, 17787-17795.	1.5	61
210	An accurate density functional theory based estimation of pKa values of polar residues combined with experimental data: from amino acids to minimal proteins. Physical Chemistry Chemical Physics, 2012, 14, 4181.	1.3	67
211	Metal-Assisted Proton Transfer in Guanine-Cytosine Pair: An Approach from Quantum Chemistry. , 2012, , .		0
212	Electronic structures of the Cu₂S₂ core of the Cu_A site in cytochrome c oxidase and nitrous oxide reductase. International Journal of Quantum Chemistry, 2012, 112, 208-218.	1.0	7
213	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn₄O₅ cluster of PSII refined to 1.9 Ã... Xâ€ray resolution. International Journal of Quantum Chemistry, 2012, 112, 253-276.	1.0	66
214	Density functional studies of the structural variety of the Cu₂S₂ core of the Cu_A site. International Journal of Quantum Chemistry, 2012, 112, 3756-3762.	1.0	0
215	Microscopic mechanisms of initial oxidation of Si(100): Reaction pathways and free-energy barriers. Physical Review B, 2012, 85, .	1.1	15
216	Full configuration interaction calculations of the second hyperpolarizabilities of the H4 model compound: Summation-over-states analysis and interplay with diradical characters. Journal of Chemical Physics, 2012, 136, 024315.	1.2	20

#	Article	IF	Citations
217	Tuned long-range corrected density functional theory method for evaluating the second hyperpolarizabilities of open-shell singlet metalâ€“metal bonded systems. Chemical Physics Letters, 2012, 523, 60-64.	1.2	10
218	Coordination effects on the electronic structure of the CuA site of cytochrome c oxidase. Chemical Physics Letters, 2012, 531, 197-201.	1.2	3
219	Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 235, 29-34.	2.0	82
220	Theoretical Studies on Metal-Containing Artificial DNA Bases. Progress in Theoretical Chemistry and Physics, 2012, , 433-460.	0.2	0
221	Density Functional Study of the Origin of the Strongly Delocalized Electronic Structure of the CuA Site in Cytochrome c Oxidase. Progress in Theoretical Chemistry and Physics, 2012, , 513-524.	0.2	0
222	First principle study of the stability of H atoms in SiN layers on MONOS-type memories during program/erase operations. , 2011, , .		3
223	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donorâ€“Acceptor Substitution. Journal of Physical Chemistry Letters, 2011, 2, 1094-1098.	2.1	111
224	Enhancement of Second Hyperpolarizabilities in Open-Shell Singlet Slipped-Stack Dimers Composed of Square Planar Nickel Complexes Involving o-Semiquinonato Type Ligands. Journal of Physical Chemistry A, 2011, 115, 1117-1124.	1.1	21
225	Theoretical Study on Reaction Scheme of Silver(I) Containing 5-Substituted Uracils Bridge Formation. Journal of Physical Chemistry A, 2011, 115, 8504-8510.	1.1	18
226	Self-diffusion in crystalline silicon: A Car-Parrinello molecular dynamics study. Physical Review B, 2011, 84, .	1.1	9
227	An Atomistic Study on Hydrogenation Effects toward Quality Improvement of Program/Erase Cycle of MONOS-Type Memory. IEICE Transactions on Electronics, 2011, E94-C, 693-698.	0.3	7
228	Collective Tunneling Model between Two-Dimensional Electron Gas to Si-Nano Dot. AIP Conference Proceedings, 2011, , .	0.3	2
229	Electron Conductivity in Modified Models of Artificial Metalâ€“DNA Using Greenâ€™s Function-Based Elastic Scattering Theory. Bulletin of the Chemical Society of Japan, 2011, 84, 366-375.	2.0	8
230	First-principles molecular dynamics study on the atomistic behavior of His503 in bovine cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 1328-1335.	0.5	2
231	Origin of the Enhancement of the Second Hyperpolarizabilities in Open-Shell Singlet Transition-Metal Systems with Metalâ€“Metal Multiple Bonds. Journal of Physical Chemistry Letters, 2011, 2, 2063-2066.	2.1	37
232	Third-Order Nonlinear Optical Properties of Open-Shell Supermolecular Systems Composed of Acetylene Linked Phenalenyl Radicals. Journal of Physical Chemistry A, 2011, 115, 8767-8777.	1.1	30
233	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. Theoretical Chemistry Accounts, 2011, 130, 711-724.	0.5	125
234	Openâ€Shell Characters and Second Hyperpolarizabilities of Oneâ€Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	1.0	46

#	Article	IF	Citations
235	A Simple scheme for estimating the pKa values of 5-substituted uracils. Chemical Physics Letters, 2011, 502, 248-252.	1.2	32
236	Molecular dynamics studies on the mutational structures of a nylon-6 byproduct-degrading enzyme. Chemical Physics Letters, 2011, 507, 157-161.	1.2	12
237	Collective Tunneling Model in Charge-Trap-Type Nonvolatile Memory Cell. Japanese Journal of Applied Physics, 2011, 50, 04DD04.	0.8	3
238	Atomistic Design of Guiding Principles for High Quality Metalâ€“Oxideâ€“Nitrideâ€“Oxideâ€“Semiconductor Memories: First Principles Study of H and O Incorporation Effects for N Vacancies in SiN Charge Trap Layers. Japanese Journal of Applied Physics, 2011, 50, 04DD05.	0.8	10
239	(Invited) Efficient Guiding Principle of Highly Scalable MONOS-Type Memories. ECS Transactions, 2011, 41, 71-79.	0.3	3
240	Study on Collective Electron Motion in Si-Nano Dot Floating Gate MOS Capacitor. IEICE Transactions on Electronics, 2011, E94.C, 730-736.	0.3	1
241	Collective Tunneling Model in Charge-Trap-Type Nonvolatile Memory Cell. Japanese Journal of Applied Physics, 2011, 50, 04DD04.	0.8	0
242	Anomalous temperature dependence of electron tunneling between a two-dimensional electron gas and Si dots. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 918-921.	1.3	0
243	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. Chemical Physics Letters, 2010, 501, 140-145.	1.2	32
244	Importance of electronic state of two-dimensional electron gas for electron injection process in nano-electronic devices. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 2602-2605.	1.3	0
245	Possibility of multi-conformational structure of mismatch DNA nucleobase in the presence of silver(I) ions. Chemical Physics Letters, 2010, 495, 125-130.	1.2	13
246	Sequenceâ€dependent protonâ€transfer reaction in stacked GC pair III: The influence of proton transfer to conductivity. International Journal of Quantum Chemistry, 2010, 110, 2221-2230.	1.0	5
247	Guiding principles for charge trap memories -A theoretical approach-. , 2010, , .		2
248	Electron Tunneling Between Si Quantum Dots and Two Dimensional Electron Gas under Optical Excitation at Low Temperatures. ECS Transactions, 2010, 28, 369-374.	0.3	0
249	Temperature Dependence of Electron Tunneling between Two Dimensional Electron Gas and Si Quantum Dots. Japanese Journal of Applied Physics, 2010, 49, 014001.	0.8	9
250	Energy Compensation Mechanism for Charge-Separated Protonation States in Aspartateâ€™Histidine Amino Acid Residue Pairs. Journal of Physical Chemistry B, 2010, 114, 6567-6578.	1.2	7
251	Effects of mercury(ii) on structural properties, electronic structure and UV absorption spectra of a duplex containing thymineâ€“mercury(ii)â€“thymine nucleobase pairs. Physical Chemistry Chemical Physics, 2010, 12, 909-917.	1.3	33
252	Universal guiding principle for the fabrication of highly scalable MONOS-type memory -atomistic recipes based on designing interface oxygen chemical potential-. , 2010, , .		5

#	Article	IF	Citations
253	Quantum Theory in Terms of Cumulant Variables. Progress in Theoretical Chemistry and Physics, 2009, , 3-34.	0.2	4
254	Effects of Hydrogen-Bonding Environments on Protonation States around the Entrance of Proton Transfer Pathways in Cytochrome c Oxidase. , 2009, , .		0
255	Electronic structure and UV absorption spectra of metal-mediate DNA: an approach from theoretical chemistry. Nucleic Acids Symposium Series, 2009, 53, 181-182.	0.3	0
256	Physics of Nano-contact between Si Quantum Dots and Inversion Layer. ECS Transactions, 2009, 25, 463-469.	0.3	9
257	Sequence dependent protonâ€transfer reaction in stacked GC pair I: The possibility of protonâ€transfer reactions. International Journal of Quantum Chemistry, 2009, 109, 2168-2177.	1.0	18
258	Theoretical studies on magnetic interactions between Cu(II) ions in hydroxypyridone nucleobases. Polyhedron, 2009, 28, 1714-1717.	1.0	9
259	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. Polyhedron, 2009, 28, 1945-1949.	1.0	12
260	Sequence-dependent proton-transfer reaction in stacked GC pair II: The origin of stabilities of proton-transfer products. Chemical Physics Letters, 2009, 478, 238-242.	1.2	20
261	Theoretical Studies on Sulfur and Metal Cation (Cu(II), Ni(II), Pd(II), and Pt(II))-Containing Artificial DNA. Journal of Physical Chemistry B, 2009, 113, 12790-12795.	1.2	8
262	Molecular Theory Including Quantum Effects and Thermal Fluctuations. Bulletin of the Chemical Society of Japan, 2009, 82, 1323-1340.	2.0	10
263	2SP6-04 First principle analyses on reaction mechanism of metalloenzyme(2SP6 Towards) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5C	0.0	0
264	Quantal cumulant dynamics III: A quantum confinement under a magnetic field. Chemical Physics Letters, 2008, 461, 310-315.	1.2	9
265	Structural Origin of Copper Ion Containing Artificial DNA: A Density Functional Study. Journal of Physical Chemistry B, 2008, 112, 16960-16965.	1.2	12
266	Single-Reference Methods for Excited States in Molecules and Polymers. Challenges and Advances in Computational Chemistry and Physics, 2008, , 15-64.	0.6	8
267	Distribution function in quantal cumulant dynamics. Journal of Chemical Physics, 2008, 128, 161103.	1.2	15
268	Correlation functions in quantized Hamilton dynamics and quantal cumulant dynamics. Journal of Chemical Physics, 2008, 129, 144104.	1.2	17
269	Dynamic Quantum Isotope Effects on Multiple Proton-Transfer Reactions. Bulletin of the Chemical Society of Japan, 2008, 81, 1230-1240.	2.0	14
270	Quantal Cumulant Dynamics for Dissipative Systems. AIP Conference Proceedings, 2008, , .	0.3	0

#	Article	IF	Citations
271	Metal-assisted proton transfer reaction in base pairs. Nucleic Acids Symposium Series, 2007, 51, 225-226.	0.3	0
272	Multiple Proton-Transfer Reactions in DNA Base Pairs by Coordination of Pt Complex. Journal of Physical Chemistry B, 2007, 111, 1176-1181.	1.2	41
273	Quantal Cumulant Dynamics for Dissipative Systems. AIP Conference Proceedings, 2007, , .	0.3	1
274	Quantal cumulant dynamics II: An efficient time-reversible integrator. Chemical Physics Letters, 2007, 443, 414-419.	1.2	14
275	Quantal cumulant dynamics: General theory. Journal of Chemical Physics, 2006, 125, 244102.	1.2	36
276	Unidirectional Electronic Ring Current Driven by a Few Cycle Circularly Polarized Laser Pulse:â€‰Quantum Model Simulations for Mgâ^Porphyrin. Journal of the American Chemical Society, 2006, 128, 7043-7049.	6.6	242
277	Influence of Pt complex binding on the guanineâ€“cytosine pair: A theoretical study. Chemical Physics Letters, 2006, 423, 331-334.	1.2	34
278	Real time mixed quantum-classical dynamics with ab initio quartic force field: Application to molecular vibrational frequency analysis. Chemical Physics Letters, 2006, 432, 585-590.	1.2	20
279	Exact-exchange time-dependent density-functional theory with the frequency-dependent kernel. Physical Review A, 2006, 73, .	1.0	30
280	Optimized effective potential method at finite temperature: An application to superconductivity. International Journal of Quantum Chemistry, 2005, 101, 774-782.	1.0	1
281	Search for the ground states of Ising spin clusters by using the genetic algorithms. International Journal of Quantum Chemistry, 2005, 105, 645-654.	1.0	5
282	Dynamic charge fluctuation of endohedral fullerene with coencapsulated Be atom and H2. Journal of Chemical Physics, 2005, 123, 131101.	1.2	16
283	Theoretical Study of the Mechanism of Hydrogenation of Side-On Coordinated Dinitrogen Activated by Zr Binuclear Complexes ([(Î·5-C5Me4H)2Zr]2(Î¼2,Î·2,Î·2-N2)). Journal of Physical Chemistry A, 2005, 109, 8800-8808.	1.1	32
284	Internal Motion of Confined Molecules in Fullerene. AIP Conference Proceedings, 2004, , .	0.3	1
285	Hybrid QM/MM studies on energetics of malonaldehyde in condensed phase. International Journal of Quantum Chemistry, 2004, 96, 32-41.	1.0	5
286	A QM/MM molecular dynamics study of a dynamical change in effective charge on Be atom in (Be+nH2)@C60. Synthetic Metals, 2003, 135-136, 765-766.	2.1	3
287	Spin and Pseudo Spins in Theoretical Chemistry. A Unified View for Superposed and Entangled Quantum Systems. Bulletin of the Korean Chemical Society, 2003, 24, 864-880.	1.0	6
288	Models for double proton and electron transfer reactions: analyses by means of quantum dynamics. Journal of Molecular Structure, 2002, 615, 267-273.	1.8	2

#	Article	IF	Citations
289	Theoretical study on triplet superconducting phase and other phases in hole-doped ferromagnetic systems. Synthetic Metals, 2001, 121, 1792-1793.	2.1	0
290	A theoretical study on conductivity of model polymer including DNA base pairs. Synthetic Metals, 2001, 119, 259-260.	2.1	5
291	Quantum spin dynamics in solution applicable to quantum computing. Journal of Molecular Liquids, 2001, 90, 63-68.	2.3	1
292	Theoretical studies on the proton and electron transfer (PET) in a pseudo one-dimensional hydrogen bonded network system. Journal of Molecular Liquids, 2001, 90, 69-74.	2.3	3
293	Calculation of quasiparticle energy of molecular systems by the GW method. International Journal of Quantum Chemistry, 2001, 84, 348-353.	1.0	5
294	Generalized spin orbital GW theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 369-374.	1.0	7
295	Non-born-oppenheimer density functional theory for excited states by using green's function techniques. International Journal of Quantum Chemistry, 2001, 84, 354-362.	1.0	1
296	Generalized spin orbital calculations of spin-frustrated molecules. International Journal of Quantum Chemistry, 2001, 84, 546-551.	1.0	14
297	Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. International Journal of Quantum Chemistry, 2001, 84, 592-600.	1.0	36
298	Electronic structure calculation by monte carlo diagonalization method. International Journal of Quantum Chemistry, 2001, 84, 601-606.	1.0	1
299	Noncollinear spin density functional theory for spin-frustrated and spin-degenerate systems. International Journal of Quantum Chemistry, 2001, 84, 670-676.	1.0	20
300	Electron propagator calculations with Kohn-Sham reference states. International Journal of Quantum Chemistry, 2001, 85, 411-420.	1.0	13
301	Theoretical studies on magnetic behavior in clusters by the genetic algorithms. International Journal of Quantum Chemistry, 2000, 80, 646-656.	1.0	4
302	Theoretical studies on superconducting and other phases: Triplet superconductivity, ferromagnetism, and ferromagnetic metal. International Journal of Quantum Chemistry, 2000, 80, 721-732.	1.0	15
303	Ab initio computations of effective exchange integrals for Hâ€“H, Hâ€“Heâ€“H and Mn2O2 complex: comparison of broken-symmetry approaches. Chemical Physics Letters, 2000, 319, 223-230.	1.2	675
304	Theoretical studies on effective spin interactions, spin alignments and macroscopic spin tunneling in polynuclear manganese and related complexes and their mesoscopic clusters. Coordination Chemistry Reviews, 2000, 198, 265-295.	9.5	133
305	Theoretical Studies on Quantum Tunneling of Spins in Cluster of Clusters. Molecular Crystals and Liquid Crystals, 2000, 342, 279-284.	0.3	0
306	Exciton Condensate in Model Dendrimers. Molecular Crystals and Liquid Crystals, 2000, 342, 273-278.	0.3	2

#	Article	IF	Citations
307	Theoretical studies on anomalous phases of photodoped systems in two-band model. Journal of Chemical Physics, 2000, 113, 11237-11244.	1.2	31
308	Quantum Spin Dynamics by Path Integral Centroid Molecular Dynamics Method. Progress of Theoretical Physics Supplement, 2000, 138, 533-534.	0.2	1
309	A theoretical study of spin level crossing induced by an external magnetic field of ring molecule magnet models. Chemical Physics Letters, 1999, 315, 441-445.	1.2	10
310	Quantum Phase Dynamics of Interaction between Photon Field and Magnetic System: Effects of Magnetic Quantum Tunnelling. Optical Review, 1999, 6, 227-231.	1.2	2
311	Theoretical studies on anomalous phases in molecular systems with external field: Possibility of photo-induced superconductivity. International Journal of Quantum Chemistry, 1999, 75, 549-561.	1.0	26
312	A formulation and numerical approach to molecular systems by the Green function method without the Bornâ€“Oppenheimer approximation. Journal of Chemical Physics, 1999, 111, 6171-6179.	1.2	60
313	Theoretical studies on anomalous phases in model plane systems of libeh3. Synthetic Metals, 1999, 103, 2651-2652.	2.1	8
314	Theoretical studies of magnetization by ab initio path integral method. Synthetic Metals, 1999, 103, 1989-1990.	2.1	1
315	Theoretical study on polarizability of ethylene by path integral method. Synthetic Metals, 1999, 101, 513.	2.1	1
316	Possibility of charge-mediated superconductors in the intermediate region of metal-insulator transitions. International Journal of Quantum Chemistry, 1998, 70, 1075-1084.	1.0	19
317	Path integral method by means of generalized coherent states and its numerical approach to molecular systems. I. Ensemble average of total energy. Journal of Chemical Physics, 1997, 107, 6283-6289.	1.2	9
318	Nonadiabatic treatment of molecular systems by the wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1261-1270.	1.0	4
319	Many-electron-wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1291-1301.	1.0	3
320	Collective Electron Tunneling Model in Si-Nano Dot Floating Gate MOS Structure. Key Engineering Materials, 0, 470, 48-53.	0.4	1
321	Quantal Cumulant Mechanics as Extended Ehrenfest Theorem. , 0, , .		0