Takao Tsuneda

List of Publications by Year
in descending order

89 papers	7,971 citations	185998 28 h-index	62479 80 g-index
92 all docs	92 docs citations	92 times ranked	6484 citing authors

#	Article	IF	Citations
1	A long-range correction scheme for generalized-gradient-approximation exchange functionals. Journal of Chemical Physics, 2001, 115, 3540-3544.	1.2	2,088
2	A long-range-corrected time-dependent density functional theory. Journal of Chemical Physics, 2004, 120, 8425-8433.	1.2	1,694
3	On Koopmansâ€™ theorem in density functional theory. Journal of Chemical Physics, 2010, 133, 174101.	1.2	367
4	Nonlinear optical property calculations by the long-range-corrected coupled-perturbed Kohnâ€“Sham method. Journal of Chemical Physics, 2005, 122, 234111.	1.2	278
5	A new one-parameter progressive Colleâ€“Salvetti-type correlation functional. Journal of Chemical Physics, 1999, 110, 10664-10678.	1.2	276
6	Long-range corrected density functional calculations of chemical reactions: Redetermination of parameter. Journal of Chemical Physics, 2007, 126, 154105.	1.2	276
7	A density functional study of van der Waals interactions. Journal of Chemical Physics, 2002, 117, 6010-6015.	1.2	255
8	An investigation of density functionals: The first-row transition metal dimer calculations. Journal of Chemical Physics, 2000, 112, 545-553.	1.2	208
9	Spectroscopic Tracking of Structural Evolution in Ultrafast Stilbene Photoisomerization. Science, 2008, 322, 1073-1077.	6.0	206
10	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. Journal of Chemical Physics, 2006, 124, 144106.	1.2	195
11	A density-functional study on Ï€-aromatic interaction: Benzene dimer and naphthalene dimer. Journal of Chemical Physics, 2005, 123, 104307.	1.2	177
12	Long-range corrected density functional study on weakly bound systems: Balanced descriptions of various types of molecular interactions. Journal of Chemical Physics, 2007, 126, 234114.	1.2	135
13	Longâ€range correction for density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 375-390.	6.2	128
14	Density Functional Theory in Quantum Chemistry. , 2014, , .		119
15	A New Mechanism for the First Carbonâ"Carbon Bond Formation in the MTG Process:â€‰ A Theoretical Study. Journal of the American Chemical Society, 1998, 120, 8222-8229.	6.6	105
16	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. Journal of Chemical Physics, 2010, 132, 094107.	1.2	82
17	Theoretical study of the excitation spectra of fiveâ€membered ring compounds: Cyclopentadiene, furan, and pyrrole. Journal of Chemical Physics, 1996, 104, 2312-2320.	1.2	80
18	Self-interaction corrections in density functional theory. Journal of Chemical Physics, 2014, 140, 18A513.	1.2	75

#	Article	IF	Citations
19	The structure of monomeric and dimeric uranyl adsorption complexes on gibbsite: A combined DFT and EXAFS study. Geochimica Et Cosmochimica Acta, 2009, 73, 5975-5988.	1.6	73
20	A new spin-polarized Colle-Salvetti-type correlation energy functional. Chemical Physics Letters, 1997, 268, 510-520.	1.2	64
21	Calculations of Alkane Energies Using Long-Range Corrected DFT Combined with Intramolecular van der Waals Correlation. Organic Letters, 2010, 12, 1440-1443.	2.4	59
22	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. Macromolecules, 2016, 49, 6621-6629.	2.2	58
23	Regional self-interaction correction of density functional theory. Journal of Computational Chemistry, 2003, 24, 1592-1598.	1.5	51
24	Electron-nucleus correlation functional for multicomponent density-functional theory. Physical Review A, 2014, 89, .	1.0	45
25	Investigation of the use of density functionals in second- and third-row transition metal dimer calculations. Journal of Computational Chemistry, 2001, 22, 1995-2009.	1.5	39
26	Long-range corrected time-dependent density functional study on fluorescence of 4,4â€²-dimethylaminobenzonitrile. Journal of Chemical Physics, 2007, 126, 034504.	1.2	37
27	Water Cluster Anions Studied by the Long-Range Corrected Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 9845-9853.	1.1	36
28	Parameter-free exchange functional. Physical Review B, 2000, 62, 15527-15531.	1.1	33
29	Reaction energetics on longâ€range corrected density functional theory: Dielsâ€“Alder reactions. Journal of Computational Chemistry, 2013, 34, 379-386.	1.5	33
30	Theoretical Investigation of the H₂O₂-Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. ACS Omega, 2017, 2, 4053-4064.	1.6	29
31	Fenton reaction mechanism generating no OH radicals in Nafion membrane decomposition. Scientific Reports, 2020, 10, 18144.	1.6	28
32	UTChem â€” A Program for ab initio Quantum Chemistry. Lecture Notes in Computer Science, 2003, , 84-95.	1.0	26
33	Theoretical Study on Molecular Property of Protactinium(V) and Uranium(VI) Oxocations:Â Why Does Protactinium(V) Form Monooxo Cations in Aqueous Solution?. Journal of Physical Chemistry A, 2006, 110, 13303-13309.	1.1	24
34	An examination of density functional theories on isomerization energy calculations of organic molecules. Theoretical Chemistry Accounts, 2011, 130, 851-857.	0.5	24
35	Density functional theory for comprehensive orbital energy calculations. Journal of Chemical Physics, 2013, 139, 064102.	1.2	24
36	A theoretical investigation on photocatalytic oxidation on the TiO2 surface. Journal of Chemical Physics, 2012, 136, 024706.	1.2	23

#	Article	IF	Citations
37	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. Computational and Theoretical Chemistry, 2005, 716, 45-60.	1.5	22
38	Theoretical investigations on geometrical and electronic structures of silver clusters. Journal of Computational Chemistry, 2019, 40, 206-211.	1.5	22
39	Theoretical and Experimental Studies on the Nearâ€Infrared Photoreaction Mechanism of a Silicon Phthalocyanine Photoimmunotherapy Dye: Photoinduced Hydrolysis by Radical Anion Generation. ChemPlusChem, 2020, 85, 1959-1963.	1.3	22
40	A reexamination of exchange energy functionals. Journal of Chemical Physics, 1999, 111, 5656-5667.	1.2	21
41	Theoretical investigations on hydrogen peroxide decomposition in aquo. Physical Chemistry Chemical Physics, 2018, 20, 24992-24999.	1.3	21
42	An efficient state-specific scheme of time-dependent density functional theory. Chemical Physics Letters, 2006, 420, 391-396.	1.2	20
43	A transversing connection between density functionals. Journal of Chemical Physics, 2001, 114, 6505-6513.	1.2	19
44	Chemical Exchange Reaction of Glycinatocopper(II) Complex in Water: A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 10403-10409.	1.1	19
45	Modified Regional Self-Interaction Correction Method Based on the Pseudospectral Methodâ€. Journal of Physical Chemistry A, 2010, 114, 8521-8528.	1.1	19
46	Reactivity index based on orbital energies. Journal of Computational Chemistry, 2014, 35, 1093-1100.	1.5	18
47	Spin-orbit relativistic long-range corrected time-dependent density functional theory for investigating spin-forbidden transitions in photochemical reactions. Journal of Chemical Physics, 2011, 135, 224106.	1.2	17
48	Chemical reaction analyses based on orbitals and orbital energies. International Journal of Quantum Chemistry, 2015, 115, 270-282.	1.0	16
49	Mechanism of H₂O₂ Decomposition by Triphenylphosphine Oxide. ACS Omega, 2018, 3, 259-265.	1.6	16
50	Modular Synthesis of Carbon-Substituted Furoxans via Radical Addition Pathway. Useful Tool for Transformation of Aliphatic Carboxylic Acids Based on â€œBuild-and-Scrapâ€•Strategy. Organic Letters, 2020, 22, 1182-1187.	2.4	16
51	Relationship between orbital energy gaps and excitation energies for longâ€chain systems. Journal of Computational Chemistry, 2016, 37, 1451-1462.	1.5	15
52	On lowâ€lying excited states of extended nanographenes. Journal of Computational Chemistry, 2017, 38, 2020-2029.	1.5	15
53	2,6-Bis(trifluoromethyl)phenylboronic Esters as Protective Groups for Diols: A Protection/Deprotection Protocol for Use under Mild Conditions. Organic Letters, 2018, 20, 6064-6068.	2.4	15
54	Roles of silver nanoclusters in surface-enhanced Raman spectroscopy. Journal of Chemical Physics, 2019, 151, 094102.	1.2	15

#	Article	IF	Citations
55	Synthesis and Synthetic Application of Chloro- and Bromofuroxans. Journal of Organic Chemistry, 2020, 85, 5959-5972.	1.7	15
56	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory. , 2005, , 507-557.		14
57	Research activities of the theoretical chemistry group at the University of Tokyo. Computational and Theoretical Chemistry, 2001, 573, 91-128.	1.5	13
58	LONG-RANGE-CORRECTED TIME-DEPENDENT DENSITY FUNCTIONAL STUDY ON ELECTRONIC SPECTRA OF FIVE-MEMBERED RING COMPOUNDS AND FREE-BASE PORPHYRIN. Journal of Theoretical and Computational Chemistry, 2006, 05, 925-944.	1.8	12
59	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. Chemical Physics Letters, 2007, 436, 30-35.	1.2	12
60	A dualâ€level stateâ€specific timeâ€dependent densityâ€functional theory. Journal of Computational Chemistry, 2008, 29, 1187-1197.	1.5	12
61	Theoretical Study on the Excess Electron Binding Mechanism in the [CH₃NO₂Â·(H₂O)_n]^{â^'} (n = 1â^'6) Anion Clusters. Journal of Physical Chemistry A, 2010, 114, 8939-8947.	1.1	12
62	The relativistic effect on energies of light elements: a RESC-BOP study. Computational and Theoretical Chemistry, 2001, 537, 63-70.	1.5	10
63	Theoretical investigation of local proton conductance in the proton exchange membranes. Chemical Physics Letters, 2014, 608, 11-16.	1.2	9
64	Density Functional Theory as a Data Science. Chemical Record, 2020, 20, 618-639.	2.9	9
65	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. Journal of Theoretical and Computational Chemistry, 2002, 01, 109-136.	1.8	8
66	An examination of density functionals on aldol, Mannich and Î±-aminoxylation reaction enthalpy calculations. Theoretical Chemistry Accounts, 2011, 130, 153-160.	0.5	8
67	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. Physical Chemistry Chemical Physics, 2018, 20, 14211-14222.	1.3	8
68	Theoretical Investigations on the Photoinduced Phase Transition Mechanism of Tetrathiafulvalene-p-chloranil. Journal of Chemical Theory and Computation, 2011, 7, 2233-2239.	2.3	7
69	Modified regional selfâ€interaction corrected timeâ€dependent density functional theory for core excitedâ€state calculations. Journal of Computational Chemistry, 2009, 30, 2583-2593.	1.5	5
70	Orbital Energy-Based Reaction Analysis of SN2 Reactions. Computation, 2016, 4, 23.	1.0	5
71	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. Journal of Physical Chemistry C, 2017, 121, 8999-9010.	1.5	5
72	On principal features of organic electrolyte molecules in lithium ion battery performance. Physical Chemistry Chemical Physics, 2019, 21, 22990-22998.	1.3	5

#	Article	IF	Citations
73	Waterâ€“oxidation mechanism of cobalt phosphate co-catalyst in artificial photosynthesis: a theoretical study. Physical Chemistry Chemical Physics, 2022, , .	1.3	4
74	One-to-One Correspondence between Reaction Pathways and Reactive Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 6901-6909.	2.3	3
75	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2005, 04, 265-280.	1.8	2
76	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. Journal of Chemical Theory and Computation, 2013, 9, 3848-3854.	2.3	2
77	Catalytic Functionalization of Hexagonal Boron Nitride for Oxidation and Epoxidation Reactions by Molecular Oxygen. Journal of Physical Chemistry C, 2021, 125, 19219-19228.	1.5	2
78	Natural reaction orbitals for characterizing electron transfer responsive to nuclear coordinate displacement. Physical Chemistry Chemical Physics, 2022, 24, 3532-3545.	1.3	2
79	Theoretical Investigations on How to Reproduce dâ€“Ï€ Bonds: Transition-Metal Cationâ€“Benzene Complex Calculations. Bulletin of the Chemical Society of Japan, 2009, 82, 1367-1371.	2.0	1
80	Relativistic Density Functional Theory. Journal of Computer Chemistry Japan, 2014, 13, 71-82.	0.0	1
81	Development of Colle-Salvetti type electron-nucleus correlation functional for MC_DFT. AIP Conference Proceedings, 2015, , .	0.3	1
82	Exchange-Correlation Functionals. , 2014, , 101-124.		1
83	Orbital Energy. , 2014, , 161-188.		1
84	Ï€-Stacking on Density Functional Theory: A Review. , 2014, , 245-270.		1
85	A New Electron-nucleus Correlation Functional forMulticomponent Density Functional Theory. Journal of Computer Chemistry Japan, 2016, 15, 143-147.	0.0	1
86	Reply to the â€˜Comment on â€œTheoretical investigations on hydrogen peroxide decomposition in aquoâ€â€™ by W. H. Koppenol, Phys. Chem. Chem. Phys., 2021, 23, DOI: 10.1039/D1CP03545B. Physical Chemistry Chemical Physics, 2021, 23, 26006-26008.	1.3	1
87	A TRANSVERSING PHYSICAL CONNECTION BETWEEN KINETIC, EXCHANGE, AND CORRELATION FUNCTIONALS. , 2002, , 684-718.		0
88	Corrections for Functionals. , 2014, , 125-160.		0
89	Appendix: Fundamental Conditions. , 2014, , 189-196.		0