Takao Tsuneda

List of Publications by Citations

87 papers	7,019 citations	29 h-index	83 g-index
92 ext. papers	7,506 ext. citations	4.1 avg, IF	5.93 L-index

#	Paper	IF	Citations
87	A long-range correction scheme for generalized-gradient-approximation exchange functionals. *Journal of Chemical Physics*, **2001**, 115, 3540-3544	3.9	1881
86	A long-range-corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2004**, 120, 8425-33	3.9	1512
85	Nonlinear optical property calculations by the long-range-corrected coupled-perturbed Kohn-Sham method. *Journal of Chemical Physics*, **2005**, 122, 234111	3.9	261
84	A new one-parameter progressive Colle-Salvetti-type correlation functional. *Journal of Chemical Physics*, **1999**, 110, 10664-10678	3.9	259
83	On Koopmans' theorem in density functional theory. *Journal of Chemical Physics*, **2010**, 133, 174101	3.9	258
82	Long-range corrected density functional calculations of chemical reactions: redetermination of parameter. *Journal of Chemical Physics*, **2007**, 126, 154105	3.9	258
81	A density functional study of van der Waals interactions. *Journal of Chemical Physics*, **2002**, 117, 6010-6015	3.9	245
80	An investigation of density functionals: The first-row transition metal dimer calculations. *Journal of Chemical Physics*, **2000**, 112, 545-553	3.9	197
79	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2006**, 124, 144106	3.9	188
78	Spectroscopic tracking of structural evolution in ultrafast stilbene photoisomerization. *Science*, **2008**, 322, 1073-7	33.3	173
77	A density-functional study on pi-aromatic interaction: benzene dimer and naphthalene dimer. *Journal of Chemical Physics*, **2005**, 123, 104307	3.9	167
76	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	3.9	133
75	Long-range correction for density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 375-390	7.9	98
74	A New Mechanism for the First Carbon−Carbon Bond Formation in the MTG Process: A Theoretical Study. *Journal of the American Chemical Society*, **1998**, 120, 8222-8229	16.4	93
73	Density Functional Theory in Quantum Chemistry **2014**,		90
72	Theoretical study of the excitation spectra of five-membered ring compounds: Cyclopentadiene, furan, and pyrrole. *Journal of Chemical Physics*, **1996**, 104, 2312-2320	3.9	75
71	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. *Journal of Chemical Physics*, **2010**, 132, 094107	3.9	74

70	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	5.5	67
69	A new spin-polarized Colle-Salvetti-type correlation energy functional. *Chemical Physics Letters*, **1997**, 268, 510-520	2.5	63
68	Calculations of alkane energies using long-range corrected DFT combined with intramolecular van der Waals correlation. *Organic Letters*, **2010**, 12, 1440-3	6.2	56
67	Self-interaction corrections in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A513	3.9	52
66	Regional self-interaction correction of density functional theory. *Journal of Computational Chemistry*, **2003**, 24, 1592-8	3.5	42
65	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. *Macromolecules*, **2016**, 49, 6621-6629	5.5	38
64	Electron-nucleus correlation functional for multicomponent density-functional theory. *Physical Review A*, **2014**, 89,	2.6	36
63	Investigation of the use of density functionals in second- and third-row transition metal dimer calculations. *Journal of Computational Chemistry*, **2001**, 22, 1995-2009	3.5	36
62	Water cluster anions studied by the long-range corrected density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 9845-53	2.8	34
61	Long-range corrected time-dependent density functional study on fluorescence of 4,4Rdimethylaminobenzonitrile. *Journal of Chemical Physics*, **2007**, 126, 034504	3.9	33
60	Parameter-free exchange functional. *Physical Review B*, **2000**, 62, 15527-15531	3.3	31
59	Reaction energetics on long-range corrected density functional theory: Diels-Alder reactions. *Journal of Computational Chemistry*, **2013**, 34, 379-86	3.5	30
58	Theoretical Investigation of the HO-Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. *ACS Omega*, **2017**, 2, 4053-4064	3.9	24
57	An examination of density functional theories on isomerization energy calculations of organic molecules. *Theoretical Chemistry Accounts*, **2011**, 130, 851-857	1.9	24
56	Theoretical study on molecular property of protactinium(V) and uranium(VI) oxocations: why does protactinium(V) form monooxo cations in aqueous solution?. *Journal of Physical Chemistry A*, **2006**, 110, 13303-9	2.8	23
55	UTChem ÐA Program for ab initio Quantum Chemistry. *Lecture Notes in Computer Science*, **2003**, 84-95	0.9	22
54	A theoretical investigation on photocatalytic oxidation on the TiO2 surface. *Journal of Chemical Physics*, **2012**, 136, 024706	3.9	21
53	Density functional theory for comprehensive orbital energy calculations. *Journal of Chemical Physics*, **2013**, 139, 064102	3.9	20

52	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. *Computational and Theoretical Chemistry*, **2005**, 716, 45-60		20
51	A reexamination of exchange energy functionals. *Journal of Chemical Physics*, **1999**, 111, 5656-5667	3.9	20
50	An efficient state-specific scheme of time-dependent density functional theory. *Chemical Physics Letters*, **2006**, 420, 391-396	2.5	19
49	Modified regional self-interaction correction method based on the pseudospectral method. *Journal of Physical Chemistry A*, **2010**, 114, 8521-8	2.8	18
48	Chemical exchange reaction of glycinatocopper(II) complex in water: a theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 10403-9	2.8	18
47	A transversing connection between density functionals. *Journal of Chemical Physics*, **2001**, 114, 6505-6513	3.9	18
46	Theoretical investigations on geometrical and electronic structures of silver clusters. *Journal of Computational Chemistry*, **2019**, 40, 206-211	3.5	17
45	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	3.9	14
44	Mechanism of HO Decomposition by Triphenylphosphine Oxide. *ACS Omega*, **2018**, 3, 259-265	3.9	13
43	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory **2005**, 507-557		13
42	Research activities of the theoretical chemistry group at the University of Tokyo. *Computational and Theoretical Chemistry*, **2001**, 573, 91-128		13
41	Theoretical and Experimental Studies on the Near-Infrared Photoreaction Mechanism of a Silicon Phthalocyanine Photoimmunotherapy Dye: Photoinduced Hydrolysis by Radical Anion Generation. *ChemPlusChem*, **2020**, 85, 1959-1963	2.8	12
40	Reactivity index based on orbital energies. *Journal of Computational Chemistry*, **2014**, 35, 1093-100	3.5	12
39	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	6.2	12
38	On low-lying excited states of extended nanographenes. *Journal of Computational Chemistry*, **2017**, 38, 2020-2029	3.5	11
37	Theoretical study on the excess electron binding mechanism in the [CH(3)NO(2).(H(2)O)(n)](-) (n = 1-6) anion clusters. *Journal of Physical Chemistry A*, **2010**, 114, 8939-47	2.8	11
36	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. *Chemical Physics Letters*, **2007**, 436, 30-35	2.5	11
35	A dual-level state-specific time-dependent density-functional theory. *Journal of Computational Chemistry*, **2008**, 29, 1187-97	3.5	11

34	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	11
33	Chemical reaction analyses based on orbitals and orbital energies. *International Journal of Quantum Chemistry*, **2015**, 115, 270-282	2.1	10
32	Modular Synthesis of Carbon-Substituted Furoxans via Radical Addition Pathway. Useful Tool for Transformation of Aliphatic Carboxylic Acids Based on "Build-and-Scrap" Strategy. *Organic Letters*, **2020**, 22, 1182-1187	6.2	10
31	The relativistic effect on energies of light elements: a RESC-BOP study. *Computational and Theoretical Chemistry*, **2001**, 537, 63-70		10
30	Synthesis and Synthetic Application of Chloro- and Bromofuroxans. *Journal of Organic Chemistry*, **2020**, 85, 5959-5972	4.2	9
29	Theoretical investigations on hydrogen peroxide decomposition in aquo. *Physical Chemistry Chemical Physics*, **2018**, 20, 24992-24999	3.6	9
28	Roles of silver nanoclusters in surface-enhanced Raman spectroscopy. *Journal of Chemical Physics*, **2019**, 151, 094102	3.9	8
27	Theoretical investigation of local proton conductance in the proton exchange membranes. *Chemical Physics Letters*, **2014**, 608, 11-16	2.5	8
26	Fenton reaction mechanism generating no OH radicals in Nafion membrane decomposition. *Scientific Reports*, **2020**, 10, 18144	4.9	8
25	Relationship between orbital energy gaps and excitation energies for long-chain systems. *Journal of Computational Chemistry*, **2016**, 37, 1451-62	3.5	8
24	An examination of density functionals on aldol, Mannich and □aminoxylation reaction enthalpy calculations. *Theoretical Chemistry Accounts*, **2011**, 130, 153-160	1.9	7
23	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. *Journal of Theoretical and Computational Chemistry*, **2002**, 01, 109-136	1.8	6
22	Theoretical Investigations on the Photoinduced Phase Transition Mechanism of Tetrathiafulvalene-p-chloranil. *Journal of Chemical Theory and Computation*, **2011**, 7, 2233-9	6.4	5
21	Modified regional self-interaction corrected time-dependent density functional theory for core excited-state calculations. *Journal of Computational Chemistry*, **2009**, 30, 2583-93	3.5	5
20	Density Functional Theory as a Data Science. *Chemical Record*, **2020**, 20, 618-639	6.6	5
19	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. *Physical Chemistry Chemical Physics*, **2018**, 20, 14211-14222	3.6	3
18	Orbital Energy-Based Reaction Analysis of SN2 Reactions. *Computation*, **2016**, 4, 23	2.2	3
17	On principal features of organic electrolyte molecules in lithium ion battery performance. *Physical Chemistry Chemical Physics*, **2019**, 21, 22990-22998	3.6	3

16	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	3.8	2
15	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. *Journal of Chemical Theory and Computation*, **2013**, 9, 3848-54	6.4	2
14	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 265-280	1.8	2
13	Relativistic Density Functional Theory. *Journal of Computer Chemistry Japan*, **2014**, 13, 71-82	0.2	1
12	Theoretical Investigations on How to Reproduce d Bonds: Transition-Metal Cation Benzene Complex Calculations. *Bulletin of the Chemical Society of Japan*, **2009**, 82, 1367-1371	5.1	1
11	One-to-One Correspondence between Reaction Pathways and Reactive Orbitals. *Journal of Chemical Theory and Computation*, **2021**, 17, 6901-6909	6.4	1
10	Exchange-Correlation Functionals **2014**, 101-124		1
9	Orbital Energy **2014**, 161-188		1
8	A New Electron-nucleus Correlation Functional for Multicomponent Density Functional Theory. *Journal of Computer Chemistry Japan*, **2016**, 15, 143-147	0.2	1
7	Quantum Chemistry **2014**, 1-33		1
6	Reply to the Comment on "Theoretical investigations on hydrogen peroxide decomposition in aquo" by W. H. Koppenol, , 2021, , DOI: 10.1039/D1CP03545B. *Physical Chemistry Chemical Physics*, **2021**, 23, 26006-26008	3.6	0
5	Stacking on Density Functional Theory: A Review **2014**, 245-270		0
4	Catalytic Functionalization of Hexagonal Boron Nitride for Oxidation and Epoxidation Reactions by Molecular Oxygen. *Journal of Physical Chemistry C*, **2021**, 125, 19219-19228	3.8	0
3	A TRANSVERSING PHYSICAL CONNECTION BETWEEN KINETIC, EXCHANGE, AND CORRELATION FUNCTIONALS **2002**, 684-718		
2	Corrections for Functionals **2014**, 125-160		
1	Appendix: Fundamental Conditions **2014**, 189-196		