

Takao Tsuneda

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Reply to the Comment on "Theoretical investigations on hydrogen peroxide decomposition in aquo" by W. H. Koppenol, , 2021, , DOI: 10.1039/D1CP03545B. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26006-26008	3.6	0
86	One-to-One Correspondence between Reaction Pathways and Reactive Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6901-6909	6.4	1
85	Catalytic Functionalization of Hexagonal Boron Nitride for Oxidation and Epoxidation Reactions by Molecular Oxygen. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19219-19228	3.8	0
84	Theoretical and Experimental Studies on the Near-Infrared Photoreaction Mechanism of a Silicon Phthalocyanine Photoimmunotherapy Dye: Photoinduced Hydrolysis by Radical Anion Generation. <i>ChemPlusChem</i> , 2020 , 85, 1959-1963	2.8	12
83	Modular Synthesis of Carbon-Substituted Furoxans via Radical Addition Pathway. Useful Tool for Transformation of Aliphatic Carboxylic Acids Based on "Build-and-Scrap" Strategy. <i>Organic Letters</i> , 2020 , 22, 1182-1187	6.2	10
82	Synthesis and Synthetic Application of Chloro- and Bromofuroxans. <i>Journal of Organic Chemistry</i> , 2020 , 85, 5959-5972	4.2	9
81	Density Functional Theory as a Data Science. <i>Chemical Record</i> , 2020 , 20, 618-639	6.6	5
80	Fenton reaction mechanism generating no OH radicals in Nafion membrane decomposition. <i>Scientific Reports</i> , 2020 , 10, 18144	4.9	8
79	Roles of silver nanoclusters in surface-enhanced Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2019 , 151, 094102	3.9	8
78	On principal features of organic electrolyte molecules in lithium ion battery performance. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22990-22998	3.6	3
77	Theoretical investigations on geometrical and electronic structures of silver clusters. <i>Journal of Computational Chemistry</i> , 2019 , 40, 206-211	3.5	17
76	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 14211-14222	3.6	3
75	Mechanism of HO Decomposition by Triphenylphosphine Oxide. <i>ACS Omega</i> , 2018 , 3, 259-265	3.9	13
74	Theoretical investigations on hydrogen peroxide decomposition in aquo. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 24992-24999	3.6	9
73	2,6-Bis(trifluoromethyl)phenylboronic Esters as Protective Groups for Diols: A Protection/Deprotection Protocol for Use under Mild Conditions. <i>Organic Letters</i> , 2018 , 20, 6064-6068	6.2	12
72	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 8999-9010	3.8	2
71	Theoretical Investigation of the HO-Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. <i>ACS Omega</i> , 2017 , 2, 4053-4064	3.9	24

70	On low-lying excited states of extended nanographenes. <i>Journal of Computational Chemistry</i> , 2017 , 38, 2020-2029	3.5	11
69	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. <i>Macromolecules</i> , 2016 , 49, 6621-6629	5.5	38
68	A New Electron-nucleus Correlation Functional for Multicomponent Density Functional Theory. <i>Journal of Computer Chemistry Japan</i> , 2016 , 15, 143-147	0.2	1
67	Orbital Energy-Based Reaction Analysis of SN2 Reactions. <i>Computation</i> , 2016 , 4, 23	2.2	3
66	Relationship between orbital energy gaps and excitation energies for long-chain systems. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1451-62	3.5	8
65	Chemical reaction analyses based on orbitals and orbital energies. <i>International Journal of Quantum Chemistry</i> , 2015 , 115, 270-282	2.1	10
64	Density Functional Theory in Quantum Chemistry 2014 ,		90
63	Long-range correction for density functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 375-390	7.9	98
62	Self-interaction corrections in density functional theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A513	3.9	52
61	Reactivity index based on orbital energies. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1093-100	3.5	12
60	Electron-nucleus correlation functional for multicomponent density-functional theory. <i>Physical Review A</i> , 2014 , 89,	2.6	36
59	Theoretical investigation of local proton conductance in the proton exchange membranes. <i>Chemical Physics Letters</i> , 2014 , 608, 11-16	2.5	8
58	Relativistic Density Functional Theory. <i>Journal of Computer Chemistry Japan</i> , 2014 , 13, 71-82	0.2	1
57	Exchange-Correlation Functionals 2014 , 101-124		1
56	Orbital Energy 2014 , 161-188		1
55	Stacking on Density Functional Theory: A Review 2014 , 245-270		0
54	Quantum Chemistry 2014 , 1-33		1
53	Corrections for Functionals 2014 , 125-160		

52 Appendix: Fundamental Conditions **2014**, 189-196

51	Density functional theory for comprehensive orbital energy calculations. <i>Journal of Chemical Physics</i> , 2013 , 139, 064102	3.9	20
50	Reaction energetics on long-range corrected density functional theory: Diels-Alder reactions. <i>Journal of Computational Chemistry</i> , 2013 , 34, 379-86	3.5	30
49	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3848-54	6.4	2
48	A theoretical investigation on photocatalytic oxidation on the TiO ₂ surface. <i>Journal of Chemical Physics</i> , 2012 , 136, 024706	3.9	21
47	Spin-orbit relativistic long-range corrected time-dependent density functional theory for investigating spin-forbidden transitions in photochemical reactions. <i>Journal of Chemical Physics</i> , 2011 , 135, 224106	3.9	14
46	An examination of density functional theories on isomerization energy calculations of organic molecules. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 851-857	1.9	24
45	An examination of density functionals on aldol, Mannich and Eminoxylation reaction enthalpy calculations. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 153-160	1.9	7
44	Theoretical Investigations on the Photoinduced Phase Transition Mechanism of Tetrathiafulvalene-p-chloranil. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2233-9	6.4	5
43	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. <i>Journal of Chemical Physics</i> , 2010 , 132, 094107	3.9	74
42	Calculations of alkane energies using long-range corrected DFT combined with intramolecular van der Waals correlation. <i>Organic Letters</i> , 2010 , 12, 1440-3	6.2	56
41	Theoretical study on the excess electron binding mechanism in the [CH(3)NO(2).(H(2)O)(n)](-) (n = 1-6) anion clusters. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8939-47	2.8	11
40	Modified regional self-interaction correction method based on the pseudospectral method. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8521-8	2.8	18
39	On Koopmans's theorem in density functional theory. <i>Journal of Chemical Physics</i> , 2010 , 133, 174101	3.9	258
38	Modified regional self-interaction corrected time-dependent density functional theory for core excited-state calculations. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2583-93	3.5	5
37	The structure of monomeric and dimeric uranyl adsorption complexes on gibbsite: A combined DFT and EXAFS study. <i>Geochimica Et Cosmochimica Acta</i> , 2009 , 73, 5975-5988	5.5	67
36	Theoretical Investigations on How to Reproduce dπ Bonds: Transition-Metal Cation-Benzene Complex Calculations. <i>Bulletin of the Chemical Society of Japan</i> , 2009 , 82, 1367-1371	5.1	1
35	Water cluster anions studied by the long-range corrected density functional theory. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 9845-53	2.8	34

34	Spectroscopic tracking of structural evolution in ultrafast stilbene photoisomerization. <i>Science</i> , 2008 , 322, 1073-7	33.3	173
33	A dual-level state-specific time-dependent density-functional theory. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1187-97	3.5	11
32	Long-range corrected time-dependent density functional study on fluorescence of 4,4Rdimethylaminobenzonitrile. <i>Journal of Chemical Physics</i> , 2007 , 126, 034504	3.9	33
31	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2007 , 436, 30-35	2.5	11
30	Long-range corrected density functional study on weakly bound systems: balanced descriptions of various types of molecular interactions. <i>Journal of Chemical Physics</i> , 2007 , 126, 234114	3.9	133
29	Long-range corrected density functional calculations of chemical reactions: redetermination of parameter. <i>Journal of Chemical Physics</i> , 2007 , 126, 154105	3.9	258
28	LONG-RANGE-CORRECTED TIME-DEPENDENT DENSITY FUNCTIONAL STUDY ON ELECTRONIC SPECTRA OF FIVE-MEMBERED RING COMPOUNDS AND FREE-BASE PORPHYRIN. <i>Journal of Theoretical and Computational Chemistry</i> , 2006 , 05, 925-944	1.8	11
27	Theoretical study on molecular property of protactinium(V) and uranium(VI) oxocations: why does protactinium(V) form monooxo cations in aqueous solution?. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 13303-9	2.8	23
26	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2006 , 124, 144106	3.9	188
25	An efficient state-specific scheme of time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2006 , 420, 391-396	2.5	19
24	Chemical exchange reaction of glycinatecopper(II) complex in water: a theoretical study. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 10403-9	2.8	18
23	Nonlinear optical property calculations by the long-range-corrected coupled-perturbed Kohn-Sham method. <i>Journal of Chemical Physics</i> , 2005 , 122, 234111	3.9	261
22	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. <i>Computational and Theoretical Chemistry</i> , 2005 , 716, 45-60		20
21	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory 2005 , 507-557		13
20	A density-functional study on pi-aromatic interaction: benzene dimer and naphthalene dimer. <i>Journal of Chemical Physics</i> , 2005 , 123, 104307	3.9	167
19	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2005 , 04, 265-280	1.8	2
18	A long-range-corrected time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2004 , 120, 8425-33	3.9	1512
17	Regional self-interaction correction of density functional theory. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1592-8	3.5	42

16	UTChem \square A Program for ab initio Quantum Chemistry. <i>Lecture Notes in Computer Science</i> , 2003 , 84-95	0.9	22
15	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2002 , 01, 109-136	1.8	6
14	A TRANSVERSING PHYSICAL CONNECTION BETWEEN KINETIC, EXCHANGE, AND CORRELATION FUNCTIONALS 2002 , 684-718		
13	A density functional study of van der Waals interactions. <i>Journal of Chemical Physics</i> , 2002 , 117, 6010-6015	3.5	245
12	Investigation of the use of density functionals in second- and third-row transition metal dimer calculations. <i>Journal of Computational Chemistry</i> , 2001 , 22, 1995-2009	3.5	36
11	The relativistic effect on energies of light elements: a RESC-BOP study. <i>Computational and Theoretical Chemistry</i> , 2001 , 537, 63-70		10
10	Research activities of the theoretical chemistry group at the University of Tokyo. <i>Computational and Theoretical Chemistry</i> , 2001 , 573, 91-128		13
9	A transversing connection between density functionals. <i>Journal of Chemical Physics</i> , 2001 , 114, 6505-6513	3.9	18
8	A long-range correction scheme for generalized-gradient-approximation exchange functionals. <i>Journal of Chemical Physics</i> , 2001 , 115, 3540-3544	3.9	1881
7	Parameter-free exchange functional. <i>Physical Review B</i> , 2000 , 62, 15527-15531	3.3	31
6	An investigation of density functionals: The first-row transition metal dimer calculations. <i>Journal of Chemical Physics</i> , 2000 , 112, 545-553	3.9	197
5	A reexamination of exchange energy functionals. <i>Journal of Chemical Physics</i> , 1999 , 111, 5656-5667	3.9	20
4	A new one-parameter progressive ColleSalvetti-type correlation functional. <i>Journal of Chemical Physics</i> , 1999 , 110, 10664-10678	3.9	259
3	A New Mechanism for the First Carbon-Carbon Bond Formation in the MTG Process: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1998 , 120, 8222-8229	16.4	93
2	A new spin-polarized Colle-Salvetti-type correlation energy functional. <i>Chemical Physics Letters</i> , 1997 , 268, 510-520	2.5	63
1	Theoretical study of the excitation spectra of five-membered ring compounds: Cyclopentadiene, furan, and pyrrole. <i>Journal of Chemical Physics</i> , 1996 , 104, 2312-2320	3.9	75