Toru Shiozaki

List of Publications by Year
in descending order

45	2,544	186265 28	233421 45
papers	citations	h-index	g-index

45	45	45	1756
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Communication: Extended multi-state complete active space second-order perturbation theory: Energy and nuclear gradients. Journal of Chemical Physics, 2011, 135, 081106.	3.0	374
2	<scp>BAGEL</scp>: Brilliantly Advanced General Electronicâ€structure Library. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1331.	14.6	164
3	Multireference explicitly correlated F12 theories. Molecular Physics, 2013, 111, 607-630.	1.7	121
4	Analytical Derivative Coupling for Multistate CASPT2 Theory. Journal of Chemical Theory and Computation, 2017, 13, 2561-2570.	5.3	109
5	Communication: Second-order multireference perturbation theory with explicit correlation: CASPT2-F12. Journal of Chemical Physics, 2010, 133, 141103.	3.0	108
6	On-the-Fly CASPT2 Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 3676-3683.	5.3	100
7	Explicitly correlated multireference configuration interaction with multiple reference functions: Avoided crossings and conical intersections. Journal of Chemical Physics, 2011, 134, 184104.	3.0	98
8	Nuclear Energy Gradients for Internally Contracted Complete Active Space Second-Order Perturbation Theory: Multistate Extensions. Journal of Chemical Theory and Computation, 2016, 12, 3781-3787.	5.3	97
9	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. Journal of Chemical Physics, 2008, 129, 071101.	3.0	94
10	Analytical energy gradients for second-order multireference perturbation theory using density fitting. Journal of Chemical Physics, 2013, 138, 104104.	3.0	93
11	Communication: Automatic code generation enables nuclear gradient computations for fully internally contracted multireference theory. Journal of Chemical Physics, 2015, 142, 051103.	3.0	91
12	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. Chemical Reviews, 2020, 120, 5878-5909.	47.7	86
13	Model Hamiltonian Analysis of Singlet Fission from First Principles. Journal of Physical Chemistry C, 2014, 118, 12700-12705.	3.1	82
14	Equations of explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3358.	2.8	77
15	Higher-order explicitly correlated coupled-cluster methods. Journal of Chemical Physics, 2009, 130, 054101.	3.0	73
16	On the difference between variational and unitary coupled cluster theories. Journal of Chemical Physics, 2018, 148, 044107.	3.0	70
17	Second- and third-order triples and quadruples corrections to coupled-cluster singles and doubles in the ground and excited states. Journal of Chemical Physics, 2007, 126, 244106.	3.0	57
18	Large-scale Diracâ€“Fockâ€“Breit method using density fitting and 2-spinor basis functions. Journal of Chemical Physics, 2013, 138, 204113.	3.0	44

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19	Anharmonic vibrational frequencies and vibrationally-averaged structures of key species in hydrocarbon combustion: HCO⁺, HCO, HNO, HOO, HOO^{â€“}, CH₃⁺, and CH₃. Molecular Physics, 2009, 107, 1283-1301.	1.7	38
20	Communication: Active space decomposition with multiple sites: Density matrix renormalization group algorithm. Journal of Chemical Physics, 2014, 141, 211102.	3.0	38
21	Fully relativistic self-consistent field under a magnetic field. Physical Chemistry Chemical Physics, 2015, 17, 14280-14283.	2.8	38
22	Communications: Explicitly correlated second-order MÃ¸llerâ€“Plesset perturbation method for extended systems. Journal of Chemical Physics, 2010, 132, 151101.	3.0	37
23	Pyrazine excited states revisited using the extended multi-state complete active space second-order perturbation method. Physical Chemistry Chemical Physics, 2013, 15, 262-269.	2.8	36
24	Fully relativistic complete active space self-consistent field for large molecules: Quasi-second-order minimax optimization. Journal of Chemical Physics, 2015, 142, 044112.	3.0	36
25	Relativistic Internally Contracted Multireference Electron Correlation Methods. Journal of Chemical Theory and Computation, 2015, 11, 4733-4739.	5.3	36
26	Explicitly correlated combined coupled-cluster and perturbation methods. Journal of Chemical Physics, 2009, 131, 044118.	3.0	33
27	Imaginary Shift in CASPT2 Nuclear Gradient and Derivative Coupling Theory. Journal of Chemical Theory and Computation, 2019, 15, 4088-4098.	5.3	30
28	Evaluation of Slater-type geminal integrals using tailored Gaussian quadrature. Chemical Physics Letters, 2009, 479, 160-164.	2.6	29
29	Quasi-diabatic States from Active Space Decomposition. Journal of Chemical Theory and Computation, 2014, 10, 3738-3744.	5.3	27
30	Large-scale relativistic complete active space self-consistent field with robust convergence. Journal of Chemical Physics, 2018, 149, 014106.	3.0	25
31	Efficient and stochastic multireference perturbation theory for large active spaces within a full configuration interaction quantum Monte Carlo framework. Journal of Chemical Physics, 2020, 152, 054101.	3.0	25
32	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. Annual Reports in Computational Chemistry, 2009, , 131-148.	1.7	24
33	Hyperfine Coupling Constants from Internally Contracted Multireference Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 4347-4351.	5.3	23
34	Communication: An efficient algorithm for evaluating the Breit and spinâ€“spin coupling integrals. Journal of Chemical Physics, 2013, 138, 111101.	3.0	19
35	On the accuracy of retinal protonated Schiff base models. Molecular Physics, 2018, 116, 2583-2590.	1.7	18
36	Analytical Nuclear Gradients of Density-Fitted Diracâ€“Fock Theory with a 2-Spinor Basis. Journal of Chemical Theory and Computation, 2013, 9, 4300-4303.	5.3	15

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37	Orbital Optimization in the Active Space Decomposition Model. Journal of Chemical Theory and Computation, 2015, 11, 3636-3642.	5.3	15
38	Visualizing Complex-Valued Molecular Orbitals. Journal of Physical Chemistry A, 2019, 123, 3223-3228.	2.5	13
39	Electronic structure of SmO and SmOâ^' via slow photoelectron velocity-map imaging spectroscopy and spin-orbit CASPT2 calculations. Journal of Chemical Physics, 2017, 147, 234311.	3.0	12
40	An efficient solver for large structured eigenvalue problems in relativistic quantum chemistry. Molecular Physics, 2017, 115, 5-12.	1.7	11
41	Numerical solution of the SinanoÇ§lu equation using a multicentre radial-angular grid. Molecular Physics, 2017, 115, 510-525.	1.7	8
42	Zero-Field Splitting Parameters from Four-Component Relativistic Methods. Journal of Chemical Theory and Computation, 2019, 15, 1560-1571.	5.3	7
43	Occupied-Orbital Fast Multipole Method for Efficient Exact Exchange Evaluation. Journal of Chemical Theory and Computation, 2018, 14, 1228-1234.	5.3	6
44	Computational Spectroscopy of the Crâ€“Cr Bond in Coordination Complexes. Inorganic Chemistry, 2021, 60, 19219-19225.	4.0	5
45	Comment on â€œA tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functionsâ€•[J. Chem. Phys. 142, 154106 (2015)]. Journal of Chemical Physics, 2020, 153, 097101.	3.0	2