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	Computational Spectroscopy of the Crâ€“Cr Bond in Coordination Complexes. Inorganic Chemistry, 2021, 60, 19219-19225.	4.0	5
2	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
3	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
4	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. Chemical Reviews, 2020, 120, 5878-5909.	47.7	86
5	Zero-Field Splitting Parameters from Four-Component Relativistic Methods. Journal of Chemical Theory and Computation, 2019, 15, 1560-1571.	5.3	7
6	Imaginary Shift in CASPT2 Nuclear Gradient and Derivative Coupling Theory. Journal of Chemical Theory and Computation, 2019, 15, 4088-4098.	5.3	30
7	Visualizing Complex-Valued Molecular Orbitals. Journal of Physical Chemistry A, 2019, 123, 3223-3228.	2.5	13
8	On the difference between variational and unitary coupled cluster theories. Journal of Chemical Physics, 2018, 148, 044107.	3.0	70
9	On the accuracy of retinal protonated Schiff base models. Molecular Physics, 2018, 116, 2583-2590.	1.7	18
10	Occupied-Orbital Fast Multipole Method for Efficient Exact Exchange Evaluation. Journal of Chemical Theory and Computation, 2018, 14, 1228-1234.	5.3	6
11	<scp>BAGEL</scp>: Brilliantly Advanced General Electronicâ€structure Library. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1331.	14.6	164
12	Large-scale relativistic complete active space self-consistent field with robust convergence. Journal of Chemical Physics, 2018, 149, 014106.	3.0	25
13	An efficient solver for large structured eigenvalue problems in relativistic quantum chemistry. Molecular Physics, 2017, 115, 5-12.	1.7	11
14	Numerical solution of the SinanoÇ§lu equation using a multicentre radial-angular grid. Molecular Physics, 2017, 115, 510-525.	1.7	8
15	Analytical Derivative Coupling for Multistate CASPT2 Theory. Journal of Chemical Theory and Computation, 2017, 13, 2561-2570.	5.3	109
16	On-the-Fly CASPT2 Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 3676-3683.	5.3	100
17	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
18	Hyperfine Coupling Constants from Internally Contracted Multireference Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 4347-4351.	5.3	23

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19	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
20	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
21	Orbital Optimization in the Active Space Decomposition Model. Journal of Chemical Theory and Computation, 2015, 11, 3636-3642.	5.3	15
22	Communication: Automatic code generation enables nuclear gradient computations for fully internally contracted multireference theory. Journal of Chemical Physics, 2015, 142, 051103.	3.0	91
23	Relativistic Internally Contracted Multireference Electron Correlation Methods. Journal of Chemical Theory and Computation, 2015, 11, 4733-4739.	5.3	36
24	Fully relativistic self-consistent field under a magnetic field. Physical Chemistry Chemical Physics, 2015, 17, 14280-14283.	2.8	38
25	Communication: Active space decomposition with multiple sites: Density matrix renormalization group algorithm. Journal of Chemical Physics, 2014, 141, 211102.	3.0	38
26	Quasi-diabatic States from Active Space Decomposition. Journal of Chemical Theory and Computation, 2014, 10, 3738-3744.	5.3	27
27	Model Hamiltonian Analysis of Singlet Fission from First Principles. Journal of Physical Chemistry C, 2014, 118, 12700-12705.	3.1	82
28	Multireference explicitly correlated F12 theories. Molecular Physics, 2013, 111, 607-630.	1.7	121
29	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
30	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
31	Analytical energy gradients for second-order multireference perturbation theory using density fitting. Journal of Chemical Physics, 2013, 138, 104104.	3.0	93
32	Communication: An efficient algorithm for evaluating the Breit and spinâ€“spin coupling integrals. Journal of Chemical Physics, 2013, 138, 111101.	3.0	19
33	Large-scale Diracâ€“Fockâ€“Breit method using density fitting and 2-spinor basis functions. Journal of Chemical Physics, 2013, 138, 204113.	3.0	44
34	Explicitly correlated multireference configuration interaction with multiple reference functions: Avoided crossings and conical intersections. Journal of Chemical Physics, 2011, 134, 184104.	3.0	98
35	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
36	Communications: Explicitly correlated second-order MÃ¸llerâ€“Plesset perturbation method for extended systems. Journal of Chemical Physics, 2010, 132, 151101.	3.0	37

#	Article	IF	Citations
37	Communication: Second-order multireference perturbation theory with explicit correlation: CASPT2-F12. Journal of Chemical Physics, 2010, 133, 141103.	3.0	108
38	Higher-order explicitly correlated coupled-cluster methods. Journal of Chemical Physics, 2009, 130, 054101.	3.0	73
39	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. Annual Reports in Computational Chemistry, 2009, , 131-148.	1.7	24
40	Evaluation of Slater-type geminal integrals using tailored Gaussian quadrature. Chemical Physics Letters, 2009, 479, 160-164.	2.6	29
41	Explicitly correlated combined coupled-cluster and perturbation methods. Journal of Chemical Physics, 2009, 131, 044118.	3.0	33
42	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
43	Equations of explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3358.	2.8	77
44	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. Journal of Chemical Physics, 2008, 129, 071101.	3.0	94
45	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