Takashi Tsuchimochi

List of Publications by Year
in descending order

28	4,075	361296 20	526166 27
papers	citations	h-index	g-index

28	28	28	4718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
3	Projected Hartreeâ€“Fock theory. Journal of Chemical Physics, 2012, 136, 164109.	1.2	191
4	What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?. Inorganic Chemistry, 2014, 53, 6386-6397.	1.9	126
5	Strong correlations via constrained-pairing mean-field theory. Journal of Chemical Physics, 2009, 131, 121102.	1.2	82
6	Excitation energies and Stokes shifts from a restricted open-shell Kohn-Sham approach. Journal of Chemical Physics, 2013, 138, 164101.	1.2	78
7	Bootstrap embedding: An internally consistent fragment-based method. Journal of Chemical Physics, 2016, 145, 074102.	1.2	51
8	Communication: ROHF theory made simple. Journal of Chemical Physics, 2010, 133, 141102.	1.2	48
9	Density matrix embedding in an antisymmetrized geminal power bath. Journal of Chemical Physics, 2015, 143, 024107.	1.2	46
10	Constrained-pairing mean-field theory. II. Exact treatment of dissociations to nondegenerate orbitals. Journal of Chemical Physics, 2009, 131, 164119.	1.2	41
11	Constrained active space unrestricted mean-field methods for controlling spin-contamination. Journal of Chemical Physics, 2011, 134, 064101.	1.2	39
12	Communication: Configuration interaction combined with spin-projection for strongly correlated molecular electronic structures. Journal of Chemical Physics, 2016, 144, 011101.	1.2	32
13	Extended MÃ¸ller-Plesset perturbation theory for dynamical and static correlations. Journal of Chemical Physics, 2014, 141, 164117.	1.2	31
14	Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities. Journal of Chemical Physics, 2010, 132, 024111.	1.2	30
15	Spin-flip configuration interaction singles with exact spin-projection: Theory and applications to strongly correlated systems. Journal of Chemical Physics, 2015, 143, 144114.	1.2	27
16	Black-Box Description of Electron Correlation with the Spin-Extended Configuration Interaction Model: Implementation and Assessment. Journal of Chemical Theory and Computation, 2016, 12, 1741-1759.	2.3	27
17	Application of the Sakuraiâ€“Sugiura projection method to coreâ€excitedâ€state calculation by timeâ€dependent density functional theory. Journal of Computational Chemistry, 2008, 29, 2311-2316.	1.5	21
18	Time-dependent projected Hartree-Fock. Journal of Chemical Physics, 2015, 142, 124103.	1.2	20

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19	Bridging Single- and Multireference Domains for Electron Correlation: Spin-Extended Coupled Electron Pair Approximation. Journal of Chemical Theory and Computation, 2017, 13, 1667-1681.	2.3	20
20	Spin-projection for quantum computation: A low-depth approach to strong correlation. Physical Review Research, 2020, 2, .	1.3	20
21	Constrained-pairing mean-field theory. IV. Inclusion of corresponding pair constraints and connection to unrestricted Hartreeâ€“Fock theory. Journal of Chemical Physics, 2010, 133, 134108.	1.2	19
22	Orbital-invariant spin-extended approximate coupled-cluster for multi-reference systems. Journal of Chemical Physics, 2018, 149, 044109.	1.2	16
23	General technique for analytical derivatives of post-projected Hartree-Fock. Journal of Chemical Physics, 2017, 146, 074104.	1.2	11
24	Second-Order Perturbation Theory with Spin-Symmetry-Projected Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2019, 15, 6688-6702.	2.3	10
25	Extending spinâ€symmetry projected coupledâ€cluster to large model spaces using an iterative nullâ€space projection technique. Journal of Computational Chemistry, 2019, 40, 265-278.	1.5	7
26	First-Principles Investigation on the Heterostructure Photocatalyst Comprising BiVO4 and Few-Layer Black Phosphorus. Journal of Physical Chemistry C, 2021, 125, 21840-21850.	1.5	2
27	Improved Description and Efficient Implementation of Spin-Projected Perturbation Theory for Practical Applications. Journal of Chemical Theory and Computation, 2021, 17, 3471-3482.	2.3	1
28	Systematic Approach to Electron Correlation via Spin-symmetry Breaking and Restoration. Molecular Science, 2020, 14, A0109.	0.2	0