Takeshi Yanai

List of Publications by Year
in descending order

44 papers	15,611 citations	331670 21 h-index	276875 41 g-index
45 all docs	45 docs citations	45 times ranked	14768 citing authors

#	Article	IF	Citations
1	Substituent and Solvent Effects on the Photoisomerization of Cinnamate Derivatives: An XMS-CASPT2 Study. Journal of Physical Chemistry A, 2022, 126, 497-505.	2.5	3
2	In Silico Analysis and Synthesis of Nafamostat Derivatives and Evaluation of Their Anti-SARS-CoV-2 Activity. Viruses, 2022, 14, 389.	3.3	2
3	Thermally Stable Array of Discrete C_{60}s on a Two-Dimensional Crystalline Adlayer of Macrocycles both in Vacuo and under Ambient Pressure. Journal of the American Chemical Society, 2022, 144, 6749-6758.	13.7	4
4	5-Thiaporphyrinium cation: effect of sulphur incorporation on excited state dynamics. Chemical Communications, 2022, , .	4.1	3
5	Machine-Learning- and Knowledge-Based Scoring Functions Incorporating Ligand and Protein Fingerprints. ACS Omega, 2022, 7, 19030-19039.	3.5	6
6	Donor–acceptor–acceptor-type near-infrared fluorophores that contain dithienophosphole oxide and boryl groups: effect of the boryl group on the nonradiative decay. Chemical Science, 2021, 12, 6333-6341.	7.4	28
7	Interpretation of Exchange Interaction through Orbital Entanglement. Journal of Physical Chemistry Letters, 2021, 12, 1268-1274.	4.6	4
8	Investigating the Nonradiative Decay Pathway in the Excited State of Silepin Derivatives: A Study with Second-Order Multireference Perturbation Wavefunction Theory. Journal of Physical Chemistry A, 2021, 125, 559-569.	2.5	2
9	Lifetimes of Be_3^{2-} and Mg_3^{2-} Cluster Dianions. Journal of Physical Chemistry A, 2021, 125, 3579-3588.	2.5	4
10	Multireference Perturbation Theory Combined with PCM and RISM Solvation Models: A Benchmark Study for Chemical Energetics. Journal of Physical Chemistry A, 2021, 125, 8324-8336.	2.5	4
11	A DMRG/CASPT2 Investigation of Metallocorroles: Quantifying Ligand Noninnocence in Archetypal 3d and 4d Element Derivatives. Jacs Au, 2021, 1, 2303-2314.	7.9	12
12	Polarization consistent basis sets using the projector augmented wave method: a renovation brought by PAW into Gaussian basis sets. Physical Chemistry Chemical Physics, 2020, 22, 27037-27052.	2.8	2
13	A multireference coupled-electron pair approximation combined with complete-active space perturbation theory in local pair-natural orbital framework. Journal of Chemical Physics, 2020, 152, 114111.	3.0	8
14	Improved RISM-CASSCF Optimization via State-Average Treatment and Damping for Characterizing Excited Molecules in Solution with Multireference Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 4865-4873.	5.3	7
15	Projector Augmented Wave Method with Gauss-Type Atomic Orbital Basis: Implementation of the Generalized Gradient Approximation and Mesh Grid Quadrature. Journal of Chemical Theory and Computation, 2020, 16, 4883-4898.	5.3	4
16	Combination of a Voronoi-Type Complex Absorbing Potential with the XMS-CASPT2 Method and Pilot Applications. Journal of Chemical Theory and Computation, 2020, 16, 2606-2616.	5.3	14
17	Artificial Neural Networks Applied as Molecular Wave Function Solvers. Journal of Chemical Theory and Computation, 2020, 16, 3513-3529.	5.3	23
18	Electronically Excited Solute Described by RISM Approach Coupled with Multireference Perturbation Theory: Vertical Excitation Energies of Bioimaging Probes. Journal of Chemical Theory and Computation, 2018, 14, 5673-5679.	5.3	13

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19	Projector Augmented Wave Method Incorporated into Gauss-Type Atomic Orbital Based Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 3236-3249.	5.3	13
20	Multistate Complete-Active-Space Second-Order Perturbation Theory Based on Density Matrix Renormalization Group Reference States. Journal of Chemical Theory and Computation, 2017, 13, 4829-4840.	5.3	48
21	Fully Internally Contracted Multireference Configuration Interaction Theory Using Density Matrix Renormalization Group: A Reduced-Scaling Implementation Derived by Computer-Aided Tensor Factorization. Journal of Chemical Theory and Computation, 2015, 11, 5120-5131.	5.3	65
22	Density matrix renormalization group for *ab initio* Calculations and associated dynamic correlation methods: A review of theory and applications. International Journal of Quantum Chemistry, 2015, 115, 283-299.	2.0	147
23	Complete active space second-order perturbation theory with cumulant approximation for extended active-space wavefunction from density matrix renormalization group. Journal of Chemical Physics, 2014, 141, 174111.	3.0	110
24	Reactivity of the Binuclear Non-Heme Iron Active Site of Î"^{9} Desaturase Studied by Large-Scale Multireference *Ab Initio* Calculations. Journal of the American Chemical Society, 2014, 136, 15977-15991.	13.7	60
25	Entangled quantum electronic wavefunctions of the Mn4CaO5 cluster in photosystem II. Nature Chemistry, 2013, 5, 660-666.	13.6	215
26	Multireference configuration interaction theory using cumulant reconstruction with internal contraction of density matrix renormalization group wave function. Journal of Chemical Physics, 2013, 139, 044118.	3.0	105
27	Second-order perturbation theory with a density matrix renormalization group self-consistent field reference function: Theory and application to the study of chromium dimer. Journal of Chemical Physics, 2011, 135, 094104.	3.0	261
28	Multireference quantum chemistry through a joint density matrix renormalization group and canonical transformation theory. Journal of Chemical Physics, 2010, 132, 024105.	3.0	148
29	A review of canonical transformation theory. International Reviews in Physical Chemistry, 2010, 29, 231-271.	2.3	86
30	Orbital optimization in the density matrix renormalization group, with applications to polyenes and Î²-carotene. Journal of Chemical Physics, 2008, 128, 144117.	3.0	288
31	Recent Progress in Relativistic Electronic Structure Theory. Recent Advances in Computational, 2004, , 221-246.	0.8	4
32	A four-index transformation in Dirac's four-component relativistic theory. Chemical Physics Letters, 2004, 388, 68-73.	2.6	46
33	A new hybrid exchangeâ€"correlation functional using the Coulomb-attenuating method (CAM-B3LYP). Chemical Physics Letters, 2004, 393, 51-57.	2.6	11,492
34	A non-orthogonal Kohn-Sham method using partially fixed molecular orbitals. Theoretical Chemistry Accounts, 2003, 110, 328-337.	1.4	2
35	A highly efficient algorithm for electron repulsion integrals over relativistic four-component Gaussian-type spinors. Journal of Chemical Physics, 2002, 116, 10122-10128.	3.0	51
36	A long-range correction scheme for generalized-gradient-approximation exchange functionals. Journal of Chemical Physics, 2001, 115, 3540-3544.	3.0	2,088

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37	A new computational scheme for the Dirac–Hartree–Fock method employing an efficient integral algorithm. Journal of Chemical Physics, 2001, 114, 6526-6538.	3.0	92
38	A new implementation of four-component relativistic density functional method for heavy-atom polyatomic systems. Journal of Chemical Physics, 2001, 115, 8267-8273.	3.0	66
39	New algorithm for electron repulsion integrals oriented to the general contraction scheme. International Journal of Quantum Chemistry, 2000, 76, 396-406.	2.0	24
40	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
41	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
42	New algorithm for electron repulsion integrals oriented to the general contraction scheme. International Journal of Quantum Chemistry, 2000, 76, 396.	2.0	1
43	Theoretical study of bifurcating reaction paths. Journal of Chemical Physics, 1997, 107, 1137-1146.	3.0	54
44	Stochastic evaluation of four-component relativistic second-order many-body perturbation energies: A potentially quadratic-scaling correlation method. Journal of Chemical Physics, 0, , .	3.0	0