Per-Ãke Malmqvist

List of Publications by Year
in descending order

54 papers	16,573 citations	76326 40 h-index	161849 54 g-index
59 all docs	59 docs citations	59 times ranked	7353 citing authors

#	Article	IF	Citations
1	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	3.0	1,689
2	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	3.3	1,485
3	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
4	The multi-state CASPT2 method. Chemical Physics Letters, 1998, 288, 299-306.	2.6	1,309
5	Main Group Atoms and Dimers Studied with a New Relativistic ANO Basis Set. Journal of Physical Chemistry A, 2004, 108, 2851-2858.	2.5	1,200
6	The restricted active space (RAS) state interaction approach with spinâ€“orbit coupling. Chemical Physics Letters, 2002, 357, 230-240.	2.6	949
7	New Relativistic ANO Basis Sets for Transition Metal Atoms. Journal of Physical Chemistry A, 2005, 109, 6575-6579.	2.5	938
8	A modified definition of the zeroth-order Hamiltonian in multiconfigurational perturbation theory (CASPT2). Chemical Physics Letters, 2004, 396, 142-149.	2.6	897
9	The CASSCF state interaction method. Chemical Physics Letters, 1989, 155, 189-194.	2.6	806
10	Multiconfiguration perturbation theory with imaginary level shift. Chemical Physics Letters, 1997, 274, 196-204.	2.6	739
11	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
12	The restricted active space followed by second-order perturbation theory method: Theory and application to the study of CuO2 and Cu2O2 systems. Journal of Chemical Physics, 2008, 128, 204109.	3.0	430
13	New Relativistic Atomic Natural Orbital Basis Sets for Lanthanide Atoms with Applications to the Ce Diatom and LuF₃. Journal of Physical Chemistry A, 2008, 112, 11431-11435.	2.5	367
14	Relativistic quantum chemistry: the multiconfigurational approach. Physical Chemistry Chemical Physics, 2004, 6, 2919.	2.8	359
15	Calculation of transition density matrices by nonunitary orbital transformations. International Journal of Quantum Chemistry, 1986, 30, 479-494.	2.0	357
16	Cholesky Decomposition-Based Multiconfiguration Second-Order Perturbation Theory (CD-CASPT2): Application to the Spin-State Energetics of Co^{III}(diiminato)(NPh). Journal of Chemical Theory and Computation, 2008, 4, 694-702.	5.3	336
17	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
18	New relativistic ANO basis sets for actinide atoms. Chemical Physics Letters, 2005, 409, 295-299.	2.6	253

#	Article	IF	Citations
19	Transition probability calculations for atoms using nonorthogonal orbitals. Physical Review E, 1995, 52, 4499-4508.	2.1	244
20	Exploring the Actinideâ^'Actinide Bond:Â Theoretical Studies of the Chemical Bond in Ac2, Th2, Pa2, and U2. Journal of the American Chemical Society, 2006, 128, 17000-17006.	13.7	179
21	How to select active space for multiconfigurational quantum chemistry?. International Journal of Quantum Chemistry, 2011, 111, 3329-3338.	2.0	178
22	Theoretical characterization of the lowest-energy absorption band of pyrrole. Journal of Chemical Physics, 2002, 116, 7526-7536.	3.0	116
23	On the Electronic Structure of the UO2 Molecule. Journal of Physical Chemistry A, 2001, 105, 10602-10606.	2.5	91
24	A theoretical study of the 1B2u and 1B1u vibronic bands in benzene. Journal of Chemical Physics, 2000, 112, 2798-2809.	3.0	87
25	Calculation of EPR g Tensors for Transitionâ€Metal Complexes Based on Multiconfigurational Perturbation Theory (CASPT2). ChemPhysChem, 2007, 8, 1803-1815.	2.1	85
26	Superior Photoprotective Motifs and Mechanisms in Eumelanins Uncovered. Journal of the American Chemical Society, 2014, 136, 11626-11635.	13.7	85
27	On the use of a Hessian model function in molecular geometry optimizations. Chemical Physics Letters, 1995, 241, 423-428.	2.6	84
28	On the inherent divergence in the MÃ¸ller-Plesset series. The neon atom â€" a test case. Chemical Physics Letters, 1996, 261, 369-378.	2.6	79
29	A theoretical study of the low-lying excited states of ozone. Chemical Physics Letters, 1995, 237, 195-203.	2.6	76
30	Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, CH2UH2. Inorganic Chemistry, 2007, 46, 4917-4925.	4.0	73
31	Franck-Condon factors for multidimensional harmonic oscillators. Chemical Physics, 1998, 228, 227-240.	1.9	65
32	Molecular integrals by numerical quadrature. I. Radial integration. Theoretical Chemistry Accounts, 2001, 106, 178-187.	1.4	64
33	Relativistic and correlated calculations on the ground and excited states of ThO. Journal of Chemical Physics, 2003, 119, 798-805.	3.0	60
34	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. Theoretical Chemistry Accounts, 2004, 112, 84-94.	1.4	59
35	Infrared Spectra and Quantum Chemical Calculations of the Uranium Carbide Molecules UC and CUC with Triple Bonds. Journal of the American Chemical Society, 2010, 132, 8484-8488.	13.7	55
36	Theoretical Study of the Lowest1BUStates oftrans-Stilbene. Journal of Physical Chemistry A, 2002, 106, 7355-7361.	2.5	52

#	Article	IF	Citations
37	Vibronic structure in triatomic molecules: The hydrocarbon flame bands of the formyl radical (HCO). A theoretical study. Journal of Chemical Physics, 1998, 108, 7202-7216.	3.0	51
38	On the low-lying singlet excited states of styrene: a theoretical contribution. Physical Chemistry Chemical Physics, 2000, 2, 2211-2217.	2.8	50
39	Potential Energy Surface of the Chromium Dimer Re-re-revisited with Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 1647-1655.	5.3	49
40	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. Molecular Physics, 2004, 102, 2207-2216.	1.7	47
41	An ab initio quantum chemical study of vertically excited singlet states of pyrimidine. Chemical Physics, 1992, 162, 359-367.	1.9	36
42	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	3.3	35
43	On the Effects of Spinâ€“Orbit Coupling on Molecular Properties: Dipole Moment and Polarizability of PbO and Spectroscopic Constants for the Ground and Excited States. Advances in Quantum Chemistry, 2004, , 37-49.	0.8	24
44	The binatural orbitals of electronic transitions. Molecular Physics, 2012, 110, 2455-2464.	1.7	17
45	A restricted active space (RAS) SCF study of the lifetime of theA 3? state of OH+. Theoretica Chimica Acta, 1991, 79, 81-92.	0.8	14
46	Electric multipole moment fluctuations in polar liquids. Journal of Chemical Physics, 2009, 130, 124521.	3.0	13
47	A non-linear approach to configuration interaction. Chemical Physics Letters, 1987, 133, 91-101.	2.6	11
48	Size inconsistency of the IOPT method. Chemical Physics Letters, 1995, 241, 429-431.	2.6	10
49	Role of electronic curve crossing of benzeneS1state in the photodissociation of aryl halides, effect of fluorination: RASSI-SO MS-CASPT2 study. International Journal of Quantum Chemistry, 2009, 109, 1962-1974.	2.0	10
50	Dissociative recombination of HeH + . I. Rovibrational spectrum of HeH Rydberg states. Theoretical Chemistry Accounts, 1998, 100, 65-77.	1.4	6
51	Experimental and Theoretical Investigation of Simple Terminal Group 6 Arsenide Asâ‰¡MF3 Molecules. Journal of Physical Chemistry A, 2009, 113, 6064-6069.	2.5	6
52	Influence of the choice of projection manifolds in the CASPT2 implementation. Molecular Physics, 2017, 115, 2077-2085.	1.7	4
53	Non-radiative decay and fragmentation in water molecules after 1a1â^'14a1 excitation and core ionization studied by electron-energy-resolved electronâ€“ion coincidence spectroscopy. Journal of Chemical Physics, 2020, 152, 074302.	3.0	2
54	A linear response approach to second-order electronic transition intensities for multiconfigurational self-consistent field wave functions. Journal of Chemical Physics, 2002, 117, 1010-1016.	3.0	1