Per-Ãke Malmqvist

List of Publications by Year
in descending order

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54	16,573	87401	182931
papers	citations	40 h-index	54 g-index

59	59	59	8200
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
2	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.	1.2	2
3	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
4	Influence of the choice of projection manifolds in the CASPT2 implementation. Molecular Physics, 2017, 115, 2077-2085.	0.8	4
5	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
6	Potential Energy Surface of the Chromium Dimer Re-re-revisited with Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 1647-1655.	2.3	49
7	Superior Photoprotective Motifs and Mechanisms in Eumelanins Uncovered. Journal of the American Chemical Society, 2014, 136, 11626-11635.	6.6	85
8	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	1.5	35
9	The binatural orbitals of electronic transitions. Molecular Physics, 2012, 110, 2455-2464.	0.8	17
10	How to select active space for multiconfigurational quantum chemistry?. International Journal of Quantum Chemistry, 2011, 111, 3329-3338.	1.0	178
11	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	1.5	1,485
12	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.	6.6	55
13	Electric multipole moment fluctuations in polar liquids. Journal of Chemical Physics, 2009, 130, 124521.	1.2	13
14	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.	1.0	10
15	Experimental and Theoretical Investigation of Simple Terminal Group 6 Arsenide Asâ‰¡MF3 Molecules. Journal of Physical Chemistry A, 2009, 113, 6064-6069.	1.1	6
16	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.	1.1	367
17	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.	2.3	336
18	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.	1.2	430

#	Article	IF	Citations
19	Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, CH2UH2. Inorganic Chemistry, 2007, 46, 4917-4925.	1.9	73
20	Calculation of EPR g Tensors for Transitionâ€Metal Complexes Based on Multiconfigurational Perturbation Theory (CASPT2). ChemPhysChem, 2007, 8, 1803-1815.	1.0	85
21	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.	6.6	179
22	New relativistic ANO basis sets for actinide atoms. Chemical Physics Letters, 2005, 409, 295-299.	1.2	253
23	New Relativistic ANO Basis Sets for Transition Metal Atoms. Journal of Physical Chemistry A, 2005, 109, 6575-6579.	1.1	938
24	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.	0.4	24
25	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. Theoretical Chemistry Accounts, 2004, 112, 84-94.	0.5	59
26	A modified definition of the zeroth-order Hamiltonian in multiconfigurational perturbation theory (CASPT2). Chemical Physics Letters, 2004, 396, 142-149.	1.2	897
27	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. Molecular Physics, 2004, 102, 2207-2216.	0.8	47
28	Main Group Atoms and Dimers Studied with a New Relativistic ANO Basis Set. Journal of Physical Chemistry A, 2004, 108, 2851-2858.	1.1	1,200
29	Relativistic quantum chemistry: the multiconfigurational approach. Physical Chemistry Chemical Physics, 2004, 6, 2919.	1.3	359
30	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	1.4	1,689
31	Relativistic and correlated calculations on the ground and excited states of ThO. Journal of Chemical Physics, 2003, 119, 798-805.	1.2	60
32	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.	1.2	1
33	Theoretical characterization of the lowest-energy absorption band of pyrrole. Journal of Chemical Physics, 2002, 116, 7526-7536.	1.2	116
34	Theoretical Study of the Lowest1BUStates oftrans-Stilbene. Journal of Physical Chemistry A, 2002, 106, 7355-7361.	1.1	52
35	The restricted active space (RAS) state interaction approach with spinâ€“orbit coupling. Chemical Physics Letters, 2002, 357, 230-240.	1.2	949
36	On the Electronic Structure of the UO2 Molecule. Journal of Physical Chemistry A, 2001, 105, 10602-10606.	1.1	91

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37	Molecular integrals by numerical quadrature. I. Radial integration. Theoretical Chemistry Accounts, 2001, 106, 178-187.	0.5	64
38	A theoretical study of the 1B2u and 1B1u vibronic bands in benzene. Journal of Chemical Physics, 2000, 112, 2798-2809.	1.2	87
39	On the low-lying singlet excited states of styrene: a theoretical contribution. Physical Chemistry Chemical Physics, 2000, 2, 2211-2217.	1.3	50
40	The multi-state CASPT2 method. Chemical Physics Letters, 1998, 288, 299-306.	1.2	1,309
41	Dissociative recombination of HeH + . I. Rovibrational spectrum of HeH Rydberg states. Theoretical Chemistry Accounts, 1998, 100, 65-77.	0.5	6
42	Franck-Condon factors for multidimensional harmonic oscillators. Chemical Physics, 1998, 228, 227-240.	0.9	65
43	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.	1.2	51
44	Multiconfiguration perturbation theory with imaginary level shift. Chemical Physics Letters, 1997, 274, 196-204.	1.2	739
45	On the inherent divergence in the MÃ¸ller-Plesset series. The neon atom â€" a test case. Chemical Physics Letters, 1996, 261, 369-378.	1.2	79
46	A theoretical study of the low-lying excited states of ozone. Chemical Physics Letters, 1995, 237, 195-203.	1.2	76
47	On the use of a Hessian model function in molecular geometry optimizations. Chemical Physics Letters, 1995, 241, 423-428.	1.2	84
48	Size inconsistency of the IOPT method. Chemical Physics Letters, 1995, 241, 429-431.	1.2	10
49	Transition probability calculations for atoms using nonorthogonal orbitals. Physical Review E, 1995, 52, 4499-4508.	0.8	244
50	An ab initio quantum chemical study of vertically excited singlet states of pyrimidine. Chemical Physics, 1992, 162, 359-367.	0.9	36
51	A restricted active space (RAS) SCF study of the lifetime of theA 3? state of OH+. Theoretica Chimica Acta, 1991, 79, 81-92.	0.9	14
52	The CASSCF state interaction method. Chemical Physics Letters, 1989, 155, 189-194.	1.2	806
53	A non-linear approach to configuration interaction. Chemical Physics Letters, 1987, 133, 91-101.	1.2	11
54	Calculation of transition density matrices by nonunitary orbital transformations. International Journal of Quantum Chemistry, 1986, 30, 479-494.	1.0	357