Sten Rettrup

List of Publications by Year in descending order

43 papers	842 citations	516710 16 h-index	477307 29 g-index
43 all docs	43 docs citations	43 times ranked	642 citing authors

#	Article	IF	Citations
1	An iterative method for calculating several of the extreme eigensolutions of large real non-symmetric matrices. Journal of Computational Physics, 1982, 45, 100-107.	3.8	133
2	A programmable spin-free method for configuration interaction. Theoretica Chimica Acta, 1977, 46, 63-71.	0.8	81
3	Large-scaleRPA calculations of chiroptical properties of organic molecules: Program RPAC. International Journal of Quantum Chemistry, 1983, 23, 595-611.	2.0	81
4	Benchmarking Second Order Methods for the Calculation of Vertical Electronic Excitation Energies: Valence and Rydberg States in Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 11995-12012.	2.5	51
5	Limited configuration interaction calculation of the optical spectrum for the permanganate ion. Chemical Physics, 1983, 74, 77-81.	1.9	46
6	Coarctate and MÃ¶bius: The Helical Orbitals of Allene and Other Cumulenes. ACS Central Science, 2018, 4, 688-700.	11.3	46
7	Two-Dimensional Model for Polymer-Based Photovoltaic Cells:Â Numerical Simulations of Morphology Effects. Journal of Physical Chemistry B, 2004, 108, 4296-4307.	2.6	45
8	Electron density of orthoboric acid determined by X-ray diffraction at 105 K and ab initio calculations. Acta Crystallographica Section B: Structural Science, 1986, 42, 545-552.	1.8	41
9	A recursive formula for Young's orthogonal representation. Chemical Physics Letters, 1977, 47, 59-60.	2.6	29
10	Two-photon absorption cross sections: An investigation of the accuracy of calculated absolute and relative values. Journal of Chemical Physics, 2006, 124, 114108.	3.0	23
11	A new symmetric group program for direct configuration interaction studies of molecules. International Journal of Quantum Chemistry, 1987, 32, 513-521.	2.0	22
12	Molecular point group adaptation of spin-free configurations. International Journal of Quantum Chemistry, 1982, 22, 127-148.	2.0	19
13	Direct evaluation of spin representation matrices and ordering of permutation-group elements. International Journal of Quantum Chemistry, 1986, 29, 119-128.	2.0	19
14	Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH2OH. Chemical Physics, 1988, 122, 45-51.	1.9	19
15	Group Theoretical Techniques and the Many-Electron Problem. Advances in Quantum Chemistry, 1981, , 125-168.	0.8	17
16	Average virtual orbitals in configuration interaction studies with application to the low-lying singlet states of the carbon monoxide and acetone molecules. International Journal of Quantum Chemistry, 1992, 44, 1045-1056.	2.0	16
17	Hartreeâ€“Fock operators to improve virtual orbitals and configuration interaction energies. Journal of Chemical Physics, 1994, 100, 5849-5856.	3.0	14
18	Efficient truncation strategies for multi-reference configuration interaction molecular energies and properties. Journal of Chemical Physics, 1998, 109, 7085-7092.	3.0	12

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19	Representations of the symmetric group generated by projected spin functions: A graphical approach. International Journal of Quantum Chemistry, 1996, 60, 91-98.	2.0	11
20	Experimental and Theoretical Investigation of the UV Spectrum and Kinetics of the Aminomethyl Radical, CH2NH2.. Acta Chemica Scandinavica, 1999, 53, 1054-1058.	0.7	10
21	Ab initio calculations of electrostatic potentials and deformation densities for a series of choline ester model systems. Theoretica Chimica Acta, 1980, 55, 267-281.	0.8	9
22	A configuration interaction (CI) procedure for the evaluation of twoâ€photon electronic transition probabilities. Program implementation with application to the A1gâ†'B2u transition of benzene. Journal of Chemical Physics, 1986, 85, 2105-2111.	3.0	9
23	A programmable spin-free method for configuration interaction. Theoretica Chimica Acta, 1977, 46, 63-71.	0.8	9
24	A program for the study of many-body correlations: matrix elements of the generators of U(n). Journal of Physics A, 1980, 13, 2267-2274.	1.6	8
25	Spin-free approach for evaluation of electronic matrix elements using character operators of ?N. International Journal of Quantum Chemistry, 1996, 60, 983-991.	2.0	8
26	A programmable procedure for generating many-particle states. Physics Letters, Section A: General, Atomic and Solid State Physics, 1980, 75, 181-182.	2.1	7
27	A graphical approach to configuration interaction studies in molecules using determinants of nonorthogonal orbitals. International Journal of Quantum Chemistry, 1991, 40, 709-717.	2.0	7
28	A permutationâ€group direct configuration interaction procedure for second order molecular properties. Program implementation with application to the Aâ€‰2Î£+âˆ'â†Xâ€‰2Î twoâ€photon transition of the OH radical. Journal of Chemical Physics, 1989, 91, 5518-5527.	3.0	6
29	Configuration interaction studies using biorthogonal approach toVB basis. International Journal of Quantum Chemistry, 1995, 53, 183-187.	2.0	6
30	On the evaluation of spin-orbit coupling matrix elements in a spin-adapted basis. International Journal of Quantum Chemistry, 1999, 73, 23-27.	2.0	6
31	A graphical approach to permutation group representations for many-electron systems. International Journal of Quantum Chemistry, 1996, 58, 637-643.	2.0	5
32	The spin-coupled description of phenylenedimethylidene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3301-3305.	1.7	5
33	A Symmetric Group Approach to the Calculation of Electronic Correlation Effects in Molecules. , 1987, , 533-546.		5
34	Spin-coupled calculations based on projected spin eigenfunctions. Theoretical Chemistry Accounts, 1998, 99, 64-67.	1.4	4
35	Alternative graphical representation of determinantal many-electron states. International Journal of Quantum Chemistry, 2006, 106, 2511-2517.	2.0	3
36	Molecular Geometry and First Electronic Transitions of MnO3Cl.. Acta Chemica Scandinavica, 1990, 44, 853-854.	0.7	3

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37	Iterative techniques for molecular CI wavefunctions. International Reviews in Physical Chemistry, 1987, 6, 385-392.	2.3	2
38	An indexing scheme for spin-free configurations of electrons. International Journal of Quantum Chemistry, 1988, 34, 445-455.	2.0	2
39	Normalization of projected spin eigenfunctions. Journal of Mathematical Chemistry, 1997, 22, 249-254.	1.5	2
40	Indexing scheme for classes of ?N; partitions ofN. International Journal of Quantum Chemistry, 1997, 64, 421-426.	2.0	1
41	On R(4) symmetries in atomic structure. Theoretica Chimica Acta, 1980, 57, 209-218.	0.8	0
42	Parallelization of the CI Program PEDICI. Advances in Quantum Chemistry, 1998, 31, 267-282.	0.8	0
43	The Permutation Group in Many-Electron Theory. , 1997, , 225-238.		0