Jeppe Olsen

List of Publications by Year in descending order

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74 papers	10,974 citations	94433 37 h-index	76900 74 g-index
81 all docs	81 docs citations	81 times ranked	5847 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Linear and nonlinear response functions for an exact state and for an MCSCF state. Journal of Chemical Physics, 1985, 82, 3235-3264.	3.0	1,014
3	Determinant based configuration interaction algorithms for complete and restricted configuration interaction spaces. Journal of Chemical Physics, 1988, 89, 2185-2192.	3.0	941
4	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	47.7	549
5	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	3.0	353
6	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	5.3	334
7	The prediction of molecular equilibrium structures by the standard electronic wave functions. Journal of Chemical Physics, 1997, 106, 6430-6440.	3.0	333
8	Passing the one-billion limit in full configuration-interaction (FCI) calculations. Chemical Physics Letters, 1990, 169, 463-472.	2.6	326
9	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	3.0	245
10	Transition probability calculations for atoms using nonorthogonal orbitals. Physical Review E, 1995, 52, 4499-4508.	2.1	244
11	Linear response calculations for large scale multiconfiguration selfâ€consistent field wave functions. Journal of Chemical Physics, 1988, 89, 3654-3661.	3.0	216
12	Quadratic response functions for a multiconfigurational selfâ€consistent field wave function. Journal of Chemical Physics, 1992, 97, 1174-1190.	3.0	209
13	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	1.9	204
14	The initial implementation and applications of a general active space coupled cluster method. Journal of Chemical Physics, 2000, 113, 7140-7148.	3.0	201
15	Surprising cases of divergent behavior in Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1996, 105, 5082-5090.	3.0	192
16	Torsional Barriers and Equilibrium Angle of Biphenyl: Reconciling Theory with Experiment. Journal of Chemical Theory and Computation, 2008, 4, 1460-1471.	5.3	189
17	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. Journal of Chemical Physics, 1992, 97, 9178-9187.	3.0	148
18	The CASSCF method: A perspective and commentary. International Journal of Quantum Chemistry, 2011, 111, 3267-3272.	2.0	146

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19	The generalized active space concept for the relativistic treatment of electron correlation. I. Kramers-restricted two-component configuration interaction. Journal of Chemical Physics, 2001, 114, 4775-4790.	3.0	137
20	The generalized active space concept for the relativistic treatment of electron correlation. II. Large-scale configuration interaction implementation based on relativistic 2- and 4-spinors and its application. Journal of Chemical Physics, 2003, 119, 2963-2971.	3.0	129
21	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	3.0	120
22	TIME-DEPENDENT RESPONSE THEORY WITH APPLICATIONS TO SELF-CONSISTENT FIELD AND MULTICONFIGURATIONAL SELF-CONSISTENT FIELD WAVE FUNCTIONS. Advanced Series in Physical Chemistry, 1995, , 857-990.	1.5	116
23	Full configuration interaction benchmarking of coupled-cluster models for the lowest singlet energy surfaces of N2. Journal of Chemical Physics, 2000, 113, 6677-6686.	3.0	109
24	SplitGAS Method for Strong Correlation and the Challenging Case of Cr₂. Journal of Chemical Theory and Computation, 2013, 9, 3375-3384.	5.3	97
25	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	3.0	90
26	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
27	Divergence in MÃ¸llerâ€“Plesset theory: A simple explanation based on a two-state model. Journal of Chemical Physics, 2000, 112, 9736-9748.	3.0	79
28	Triplet excitation energies in full configuration interaction and coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 3015-3020.	3.0	76
29	A general coupled cluster study of the N2 molecule. Chemical Physics Letters, 2001, 344, 578-586.	2.6	71
30	Large multiconfiguration Hartreeâ€“Fock calculations on the hyperfine structure of B(2P) and the nuclear quadrupole moments of10B and11B. Journal of Chemical Physics, 1991, 94, 5051-5055.	3.0	65
31	Triplet excitation properties in large scale multiconfiguration linear response calculations. Journal of Chemical Physics, 1989, 91, 381-388.	3.0	56
32	A relativistic 4-component general-order multi-reference coupled cluster method: initial implementation and application to HBr. Theoretical Chemistry Accounts, 2007, 118, 347-356.	1.4	55
33	Finite element multiconfiguration Hartreeâ€“Fock determination of the nuclear quadrupole moments of chlorine, potassium, and calcium isotopes. Journal of Chemical Physics, 1993, 98, 7152-7158.	3.0	49
34	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. Theoretica Chimica Acta, 1995, 90, 441-458.	0.8	46
35	An analysis and implementation of a general coupled cluster approach to excitation energies with application to the B2 molecule. Journal of Chemical Physics, 2001, 115, 671-679.	3.0	45
36	Second-Order Perturbation Theory for Generalized Active Space Self-Consistent-Field Wave Functions. Journal of Chemical Theory and Computation, 2016, 12, 3208-3213.	5.3	44

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37	The exactness of the extended Koopmansâ€™ theorem: A numerical study. Journal of Chemical Physics, 1993, 98, 3999-4002.	3.0	39
38	The hyperpolarizability dispersion of neon is not anomalous. Chemical Physics Letters, 1991, 187, 387-390.	2.6	37
39	Novel methods for configuration interaction and orbital optimization for wave functions containing non-orthogonal orbitals with applications to the chromium dimer and trimer. Journal of Chemical Physics, 2015, 143, 114102.	3.0	36
40	A direct implementation of the second-order derivatives of multiconfigurational SCF energies and an analysis of the preconditioning in the associated response equation. Molecular Physics, 1999, 96, 617-628.	1.7	31
41	On the divergent behavior of MÃ¸llerâ€“Plesset perturbation theory for the molecular electric dipole moment. Journal of Chemical Physics, 2000, 112, 1107-1112.	3.0	30
42	Quadratic Response Functions in a Second-Order Polarization Propagator Frameworkâ€. Journal of Physical Chemistry A, 2005, 109, 11618-11628.	2.5	29
43	Molecular response properties from a Hermitian eigenvalue equation for a time-periodic Hamiltonian. Journal of Chemical Physics, 2015, 142, 114109.	3.0	29
44	Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective. Journal of Chemical Physics, 2016, 144, 024102.	3.0	29
45	Spinor optimization for a relativistic spin-dependent CASSCF program. Theoretical Chemistry Accounts, 1997, 97, 125-135.	1.4	24
46	CC3 triplet excitation energies using an explicit spin coupled excitation space. Journal of Chemical Physics, 2001, 115, 3545-3552.	3.0	24
47	Cluster perturbation theory. I. Theoretical foundation for a coupled cluster target state and ground-state energies. Journal of Chemical Physics, 2019, 150, 134108.	3.0	22
48	An efficient algorithm for solving nonlinear equations with a minimal number of trial vectors: Applications to atomic-orbital based coupled-cluster theory. Journal of Chemical Physics, 2008, 128, 204105.	3.0	21
49	Cluster perturbation theory. II. Excitation energies for a coupled cluster target state. Journal of Chemical Physics, 2019, 150, 134109.	3.0	21
50	Update methods in multiconfigurational selfâ€consistent field calculations. Journal of Chemical Physics, 1982, 77, 6109-6130.	3.0	19
51	A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation. Journal of Chemical Physics, 2016, 144, 064103.	3.0	18
52	Non-orthogonal internally contracted multi-configurational perturbation theory (NICPT): Dynamic electron correlation for large, compact active spaces. Journal of Chemical Physics, 2017, 147, 174106.	3.0	18
53	Equation-of-motion coupled cluster perturbation theory revisited. Journal of Chemical Physics, 2014, 140, 174114.	3.0	17
54	Cluster perturbation theory. III. Perturbation series for coupled cluster singles and doubles excitation energies. Journal of Chemical Physics, 2019, 150, 134110.	3.0	17

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55	Divergent behavior of Mo/llerâ€“Plesset perturbation theory for molecular electric dipole and quadrupole moments. Journal of Chemical Physics, 1999, 110, 7127-7128.	3.0	16
56	A multiconfiguration selfâ€consistentâ€field response study of oneâ€and twoâ€photon dipole transitions between the Xâ€‰1Î£+ and Aâ€‰1Î states of CO. Journal of Chemical Physics, 1995, 102, 4143-4150.	3.0	15
57	Cluster perturbation theory. IV. Convergence of cluster perturbation series for energies and molecular properties. Journal of Chemical Physics, 2019, 150, 134111.	3.0	14
58	Attosecond electronic dynamics of core-excited states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> in the soft x-ray region. Physical Review Research, 2021, 3, .	3.6	14
59	Response to â€˜â€˜Comment on â€˜The exactness of the extended Koopmansâ€™ theorem: A numerical studyâ€™â€™ [J. Chem. Phys. 99, 6221 (1993)]. Journal of Chemical Physics, 1993, 99, 6222-6223.	3.0	13
60	Robust and Reliable Multilevel Minimization of the Kohnâ^'Sham Energy. Journal of Chemical Theory and Computation, 2009, 5, 1027-1032.	5.3	12
61	Convergence patterns and rates in two-state perturbation expansions. Journal of Chemical Physics, 2019, 151, 084108.	3.0	11
62	Cluster perturbation theory. V. Theoretical foundation for cluster linear target states. Journal of Chemical Physics, 2019, 150, 134112.	3.0	11
63	Dynamic correlation for non-orthogonal reference states: Improved perturbational and variational methods. Journal of Chemical Physics, 2018, 149, 144104.	3.0	9
64	Cluster perturbation theory. VI. Ground-state energy series using the Lagrangian. Journal of Chemical Physics, 0, , .	3.0	9
65	A direct method to transform between expansions in the configuration state function and Slater determinant bases. Journal of Chemical Physics, 2014, 141, 034112.	3.0	8
66	Generalising localisation schemes of orthogonal orbitals to the localisation of non-orthogonal orbitals. Molecular Physics, 2017, 115, 16-25.	1.7	8
67	Second- and higher-order convergence in linear and nonlinear multiconfigurational Hartree-Fock theory. International Journal of Quantum Chemistry, 1983, 24, 25-60.	2.0	7
68	Cluster Perturbation Theory. VII. The convergence of Cluster Perturbation Expansions. Journal of Chemical Physics, 0, , .	3.0	7
69	Convergence of coupled cluster perturbation theory. Journal of Chemical Physics, 2016, 145, 224104.	3.0	6
70	Cluster perturbation theory. VIII. First order properties for a coupled cluster state. Journal of Chemical Physics, 0, , .	3.0	5
71	The energy, orbitals and electric properties of the ozone molecule with ensemble density functional theory. Molecular Physics, 2013, 111, 1259-1270.	1.7	4
72	The evaluation of MCRPA (MCTDHF) electronic excitation energies, oscillator strengths, and polarizabilities: Application to O2. International Journal of Quantum Chemistry, 1981, 20, 151-162.	2.0	3

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73	Collecting all intermediates with an optimal scaling for the generalised-active-space coupled-cluster method with application to SbH. Molecular Physics, 2017, 115, 90-108.	1.7	2
74	A direct implementation of the second-order derivatives of multiconfigurational SCF energies and an analysis of the preconditioning in the associated response equation. Molecular Physics, 1999, 96, 617-628.	1.7	1