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	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
2	Convergence patterns and rates in two-state perturbation expansions. Journal of Chemical Physics, 2019, 151, 084108.	3.0	11
3	Cluster perturbation theory. V. Theoretical foundation for cluster linear target states. Journal of Chemical Physics, 2019, 150, 134112.	3.0	11
4	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
5	Cluster perturbation theory. III. Perturbation series for coupled cluster singles and doubles excitation energies. Journal of Chemical Physics, 2019, 150, 134110.	3.0	17
6	Cluster perturbation theory. II. Excitation energies for a coupled cluster target state. Journal of Chemical Physics, 2019, 150, 134109.	3.0	21
7	Cluster perturbation theory. IV. Convergence of cluster perturbation series for energies and molecular properties. Journal of Chemical Physics, 2019, 150, 134111.	3.0	14
8	Dynamic correlation for non-orthogonal reference states: Improved perturbational and variational methods. Journal of Chemical Physics, 2018, 149, 144104.	3.0	9
9	Generalising localisation schemes of orthogonal orbitals to the localisation of non-orthogonal orbitals. Molecular Physics, 2017, 115, 16-25.	1.7	8
10	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
11	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
12	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	3.0	120
13	Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective. Journal of Chemical Physics, 2016, 144, 024102.	3.0	29
14	Convergence of coupled cluster perturbation theory. Journal of Chemical Physics, 2016, 145, 224104.	3.0	6
15	A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation. Journal of Chemical Physics, 2016, 144, 064103.	3.0	18
16	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
17	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
18	Molecular response properties from a Hermitian eigenvalue equation for a time-periodic Hamiltonian. Journal of Chemical Physics, 2015, 142, 114109.	3.0	29

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19	Equation-of-motion coupled cluster perturbation theory revisited. Journal of Chemical Physics, 2014, 140, 174114.	3.0	17
20	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
21	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
22	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	5.3	334
23	SplitGAS Method for Strong Correlation and the Challenging Case of Cr₂. Journal of Chemical Theory and Computation, 2013, 9, 3375-3384.	5.3	97
24	The energy, orbitals and electric properties of the ozone molecule with ensemble density functional theory. Molecular Physics, 2013, 111, 1259-1270.	1.7	4
25	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	47.7	549
26	The CASSCF method: A perspective and commentary. International Journal of Quantum Chemistry, 2011, 111, 3267-3272.	2.0	146
27	Robust and Reliable Multilevel Minimization of the Kohnâ^'Sham Energy. Journal of Chemical Theory and Computation, 2009, 5, 1027-1032.	5.3	12
28	Torsional Barriers and Equilibrium Angle of Biphenyl: Reconciling Theory with Experiment. Journal of Chemical Theory and Computation, 2008, 4, 1460-1471.	5.3	189
29	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
30	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
31	Quadratic Response Functions in a Second-Order Polarization Propagator Frameworkâ€. Journal of Physical Chemistry A, 2005, 109, 11618-11628.	2.5	29
32	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	1.9	204
33	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
34	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	3.0	245
35	A general coupled cluster study of the N2 molecule. Chemical Physics Letters, 2001, 344, 578-586.	2.6	71
36	Triplet excitation energies in full configuration interaction and coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 3015-3020.	3.0	76

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37	CC3 triplet excitation energies using an explicit spin coupled excitation space. Journal of Chemical Physics, 2001, 115, 3545-3552.	3.0	24
38	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
39	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	3.0	353
40	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
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	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
43	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
44	The initial implementation and applications of a general active space coupled cluster method. Journal of Chemical Physics, 2000, 113, 7140-7148.	3.0	201
45	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
46	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
47	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
48	The prediction of molecular equilibrium structures by the standard electronic wave functions. Journal of Chemical Physics, 1997, 106, 6430-6440.	3.0	333
49	Spinor optimization for a relativistic spin-dependent CASSCF program. Theoretical Chemistry Accounts, 1997, 97, 125-135.	1.4	24
50	Surprising cases of divergent behavior in Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1996, 105, 5082-5090.	3.0	192
51	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
52	Transition probability calculations for atoms using nonorthogonal orbitals. Physical Review E, 1995, 52, 4499-4508.	2.1	244
53	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
54	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. Theoretica Chimica Acta, 1995, 90, 441-458.	0.8	46

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55	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
56	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
57	The exactness of the extended Koopmansâ€™ theorem: A numerical study. Journal of Chemical Physics, 1993, 98, 3999-4002.	3.0	39
58	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
59	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	3.0	90
60	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
61	Quadratic response functions for a multiconfigurational selfâ€consistent field wave function. Journal of Chemical Physics, 1992, 97, 1174-1190.	3.0	209
62	The hyperpolarizability dispersion of neon is not anomalous. Chemical Physics Letters, 1991, 187, 387-390.	2.6	37
63	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
64	Passing the one-billion limit in full configuration-interaction (FCI) calculations. Chemical Physics Letters, 1990, 169, 463-472.	2.6	326
65	Triplet excitation properties in large scale multiconfiguration linear response calculations. Journal of Chemical Physics, 1989, 91, 381-388.	3.0	56
66	Determinant based configuration interaction algorithms for complete and restricted configuration interaction spaces. Journal of Chemical Physics, 1988, 89, 2185-2192.	3.0	941
67	Linear response calculations for large scale multiconfiguration selfâ€consistent field wave functions. Journal of Chemical Physics, 1988, 89, 3654-3661.	3.0	216
68	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
69	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
70	Update methods in multiconfigurational selfâ€consistent field calculations. Journal of Chemical Physics, 1982, 77, 6109-6130.	3.0	19
71	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
72	Cluster perturbation theory. VI. Ground-state energy series using the Lagrangian. Journal of Chemical Physics, 0, , .	3.0	9

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73	Cluster Perturbation Theory. VII. The convergence of Cluster Perturbation Expansions. Journal of Chemical Physics, 0, , .	3.0	7
74	Cluster perturbation theory. VIII. First order properties for a coupled cluster state. Journal of Chemical Physics, 0, , .	3.0	5