Jeppe Olsen

List of Publications by Citations

71 papers	9,486 citations	36 h-index	81 g-index
81 ext. papers	10,192 ext. citations	4.5 avg, IF	5.91 L-index

#	Paper	IF	Citations
71	**2000**,		1575
70	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
69	Linear and nonlinear response functions for an exact state and for an MCSCF state. *Journal of Chemical Physics*, **1985**, 82, 3235-3264	3.9	943
68	Determinant based configuration interaction algorithms for complete and restricted configuration interaction spaces. *Journal of Chemical Physics*, **1988**, 89, 2185-2192	3.9	822
67	Recent advances in wave function-based methods of molecular-property calculations. *Chemical Reviews*, **2012**, 112, 543-631	68.1	453
66	The accurate determination of molecular equilibrium structures. *Journal of Chemical Physics*, **2001**, 114, 6548-6556	3.9	322
65	The prediction of molecular equilibrium structures by the standard electronic wave functions. *Journal of Chemical Physics*, **1997**, 106, 6430-6440	3.9	310
64	Passing the one-billion limit in full configuration-interaction (FCI) calculations. *Chemical Physics Letters*, **1990**, 169, 463-472	2.5	292
63	Multiconfiguration Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 3669-80	6.4	246
62	Molecular equilibrium structures from experimental rotational constants and calculated vibration□otation interaction constants. *Journal of Chemical Physics*, **2002**, 116, 6482-6496	3.9	222
61	Transition probability calculations for atoms using nonorthogonal orbitals. *Physical Review E*, **1995**, 52, 4499-4508	2.4	220
60	Linear response calculations for large scale multiconfiguration self-consistent field wave functions. *Journal of Chemical Physics*, **1988**, 89, 3654-3661	3.9	202
59	A priori calculation of molecular properties to chemical accuracy. *Journal of Physical Organic Chemistry*, **2004**, 17, 913-933	2.1	194
58	Quadratic response functions for a multiconfigurational self-consistent field wave function. *Journal of Chemical Physics*, **1992**, 97, 1174-1190	3.9	193
57	The initial implementation and applications of a general active space coupled cluster method. *Journal of Chemical Physics*, **2000**, 113, 7140-7148	3.9	186
56	Surprising cases of divergent behavior in Mo/ller□lesset perturbation theory. *Journal of Chemical Physics*, **1996**, 105, 5082-5090	3.9	175
55	Torsional Barriers and Equilibrium Angle of Biphenyl: Reconciling Theory with Experiment. *Journal of Chemical Theory and Computation*, **2008**, 4, 1460-71	6.4	169

54	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. *Journal of Chemical Physics*, **1992**, 97, 9178-9187	3.9	139
53	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		108
52	Full configuration interaction benchmarking of coupled-cluster models for the lowest singlet energy surfaces of N2. *Journal of Chemical Physics*, **2000**, 113, 6677-6686	3.9	104
51	The CASSCF method: A perspective and commentary. *International Journal of Quantum Chemistry*, **2011**, 111, 3267-3272	2.1	101
50	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	3.9	101
49	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	3.9	94
48	SplitGAS Method for Strong Correlation and the Challenging Case of Cr2. *Journal of Chemical Theory and Computation*, **2013**, 9, 3375-84	6.4	86
47	Spin□orbit coupling constants in a multiconfiguration linear response approach. *Journal of Chemical Physics*, **1992**, 96, 2118-2126	3.9	86
46	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. *Journal of Chemical Physics*, **2017**, 147, 184111	3.9	83
45	On the inherent divergence in the M□ller-Plesset series. The neon atom □a test case. *Chemical Physics Letters*, **1996**, 261, 369-378	2.5	74
44	Triplet excitation energies in full configuration interaction and coupled-cluster theory. *Journal of Chemical Physics*, **2001**, 115, 3015-3020	3.9	72
43	Divergence in M□ller□Plesset theory: A simple explanation based on a two-state model. *Journal of Chemical Physics*, **2000**, 112, 9736-9748	3.9	71
42	A general coupled cluster study of the N2 molecule. *Chemical Physics Letters*, **2001**, 344, 578-586	2.5	67
41	Large multiconfiguration Hartree□Fock calculations on the hyperfine structure of B(2P) and the nuclear quadrupole moments of 10B and 11B. *Journal of Chemical Physics*, **1991**, 94, 5051-5055	3.9	65
40	Triplet excitation properties in large scale multiconfiguration linear response calculations. *Journal of Chemical Physics*, **1989**, 91, 381-388	3.9	51
39	Finite element multiconfiguration Hartree□Fock determination of the nuclear quadrupole moments of chlorine, potassium, and calcium isotopes. *Journal of Chemical Physics*, **1993**, 98, 7152-7158	3.9	48
38	A relativistic 4-component general-order multi-reference coupled cluster method: initial implementation and application to HBr. *Theoretical Chemistry Accounts*, **2007**, 118, 347-356	1.9	47
37	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	3.9	41

36	Second-Order Perturbation Theory for Generalized Active Space Self-Consistent-Field Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 3208-13	6.4	39
35	The hyperpolarizability dispersion of neon is not anomalous. *Chemical Physics Letters*, **1991**, 187, 387-390	2.5	36
34	The exactness of the extended Koopmans theorem: A numerical study. *Journal of Chemical Physics*, **1993**, 98, 3999-4002	3.9	34
33	On the divergent behavior of Mller Plesset perturbation theory for the molecular electric dipole moment. *Journal of Chemical Physics*, **2000**, 112, 1107-1112	3.9	30
32	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	3.9	29
31	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	27
30	Quadratic response functions in a second-order polarization propagator framework. *Journal of Physical Chemistry A*, **2005**, 109, 11618-28	2.8	26
29	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. *Theoretica Chimica Acta*, **1995**, 90, 441-458		26
28	CC3 triplet excitation energies using an explicit spin coupled excitation space. *Journal of Chemical Physics*, **2001**, 115, 3545-3552	3.9	23
27	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	3.9	20
26	Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective. *Journal of Chemical Physics*, **2016**, 144, 024102	3.9	19
25	Spinor optimization for a relativistic spin-dependent CASSCF program. *Theoretical Chemistry Accounts*, **1997**, 97, 125-135	1.9	18
24	Update methods in multiconfigurational self-consistent field calculations. *Journal of Chemical Physics*, **1982**, 77, 6109-6130	3.9	18
23	Molecular response properties from a Hermitian eigenvalue equation for a time-periodic Hamiltonian. *Journal of Chemical Physics*, **2015**, 142, 114109	3.9	17
22	Divergent behavior of Mo/ller Plesset perturbation theory for molecular electric dipole and quadrupole moments. *Journal of Chemical Physics*, **1999**, 110, 7127-7128	3.9	16
21	A multiconfiguration self-consistent-field response study of one- and two-photon dipole transitions between the X 1 and A 1 states of CO. *Journal of Chemical Physics*, **1995**, 102, 4143-4150	3.9	15
20	Non-orthogonal internally contracted multi-configurational perturbation theory (NICPT): Dynamic electron correlation for large, compact active spaces. *Journal of Chemical Physics*, **2017**, 147, 174106	3.9	14
19	Equation-of-motion coupled cluster perturbation theory revisited. *Journal of Chemical Physics*, **2014** , 140, 174114	3.9	14

18	Cluster perturbation theory. I. Theoretical foundation for a coupled cluster target state and ground-state energies. *Journal of Chemical Physics*, **2019**, 150, 134108	3.9	12
17	Robust and Reliable Multilevel Minimization of the Kohn-Sham Energy. *Journal of Chemical Theory and Computation*, **2009**, 5, 1027-32	6.4	12
16	Response to Comment on The exactness of the extended Koopmans theorem: A numerical study[J. Chem. Phys. 99, 6221 (1993)]. *Journal of Chemical Physics*, **1993**, 99, 6222-6223	3.9	11
15	A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation. *Journal of Chemical Physics*, **2016**, 144, 064103	3.9	11
14	Cluster perturbation theory. II. Excitation energies for a coupled cluster target state. *Journal of Chemical Physics*, **2019**, 150, 134109	3.9	10
13	Generalising localisation schemes of orthogonal orbitals to the localisation of non-orthogonal orbitals. *Molecular Physics*, **2017**, 115, 16-25	1.7	7
12	Cluster perturbation theory. III. Perturbation series for coupled cluster singles and doubles excitation energies. *Journal of Chemical Physics*, **2019**, 150, 134110	3.9	7
11	Second- and higher-order convergence in linear and nonlinear multiconfigurational Hartree Fock theory. *International Journal of Quantum Chemistry*, **1983**, 24, 25-60	2.1	7
10	Cluster perturbation theory. IV. Convergence of cluster perturbation series for energies and molecular properties. *Journal of Chemical Physics*, **2019**, 150, 134111	3.9	6
9	Convergence of coupled cluster perturbation theory. *Journal of Chemical Physics*, **2016**, 145, 224104	3.9	6
8	Convergence patterns and rates in two-state perturbation expansions. *Journal of Chemical Physics*, **2019**, 151, 084108	3.9	5
7	Cluster perturbation theory. V. Theoretical foundation for cluster linear target states. *Journal of Chemical Physics*, **2019**, 150, 134112	3.9	5
6	A direct method to transform between expansions in the configuration state function and Slater determinant bases. *Journal of Chemical Physics*, **2014**, 141, 034112	3.9	5
5	Dynamic correlation for non-orthogonal reference states: Improved perturbational and variational methods. *Journal of Chemical Physics*, **2018**, 149, 144104	3.9	5
4	The energy, orbitals and electric properties of the ozone molecule with ensemble density functional theory. *Molecular Physics*, **2013**, 111, 1259-1270	1.7	4
3	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	1
2	A direct implementation of the second-order derivatives of multiconfigurational SCF energies and an analysis of the preconditioning in the associated response equation		1
1	The evaluation of MCRPA (MCTDHF) electronic excitation energies, oscillator strengths, and polarizabilities: Application to O2. *International Journal of Quantum Chemistry*, **2009**, 20, 151-162	2.1	0