Agnes Szabados

List of Publications by Year in descending order

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78 papers	1,315 citations	394421 19 h-index	395702 33 g-index
82 all docs	82 docs citations	82 times ranked	766 citing authors

#	Article	IF	Citations
1	Theoretical interpretation of Grimmeâ€™s spin-component-scaled second order MÃ¸ller-Plesset theory. Journal of Chemical Physics, 2006, 125, 214105.	3.0	88
2	On the perturbation of multiconfiguration wave functions. Journal of Chemical Physics, 2003, 119, 1922-1928.	3.0	82
3	Strongly orthogonal geminals: size-extensive and variational reference states. Journal of Mathematical Chemistry, 2012, 50, 534-551.	1.5	68
4	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
5	Intershell interaction in double walled carbon nanotubes: Charge transfer and orbital mixing. Physical Review B, 2008, 77, .	3.2	61
6	Multiconfiguration perturbation theory: Size consistency at second order. Journal of Chemical Physics, 2005, 122, 114104.	3.0	54
7	Generalized MÃ¸llerâ€“Plesset Partitioning in Multiconfiguration Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 2024-2033.	5.3	53
8	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
9	Partitioning in multiconfiguration perturbation theory. Annalen Der Physik, 2004, 13, 223-231.	2.4	45
10	Optimized partitioning in perturbation theory: Comparison to related approaches. Journal of Chemical Physics, 2000, 112, 4438-4446.	3.0	43
11	Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: Role of Dispersive Interactions. Journal of Chemical Theory and Computation, 2013, 9, 2602-2608.	5.3	42
12	Intertube interactions in carbon nanotube bundles. Physical Review B, 2006, 73, .	3.2	41
13	Perspectives of APSGâ€based multireference perturbation theories. International Journal of Quantum Chemistry, 2014, 114, 1048-1052.	2.0	39
14	Molecular Structure of Carbene Analogues:Â A Computational Study. Journal of Physical Chemistry A, 2003, 107, 4314-4321.	2.5	35
15	Optimized partitioning in Rayleighâ€“SchrÃ¶dinger perturbation theory. Chemical Physics Letters, 1999, 308, 303-309.	2.6	34
16	Semiconductor-to-metal transition of double walled carbon nanotubes induced by inter-shell interaction. Physica Status Solidi (B): Basic Research, 2006, 243, 3476-3479.	1.5	30
17	A sparse matrix based full-configuration interaction algorithm. Journal of Chemical Physics, 2008, 128, 144101.	3.0	26
18	Sensitivity analysis of state-specific multireference perturbation theory. Journal of Chemical Physics, 2011, 134, 174113.	3.0	23

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19	Local spin from strongly orthogonal geminal wavefunctions. Molecular Physics, 2015, 113, 249-259.	1.7	23
20	Bilinear Constraints upon the Correlation Contribution to the Electronâ€“Electron Repulsion Energy as a Functional of the One-Electron Reduced Density Matrix. Journal of Chemical Theory and Computation, 2019, 15, 4862-4872.	5.3	19
21	Damping of perturbation corrections in quasidegenerate situations. Journal of Chemical Physics, 1996, 104, 3320-3324.	3.0	16
22	On the â€œkiller conditionâ€™' in the equation-of-motion method: ionization potentials from multi-reference wave functions. Physical Chemistry Chemical Physics, 2001, 3, 696-701.	2.8	15
23	Spin Symmetry and Size Consistency of Strongly Orthogonal Geminals. Journal of Chemical Theory and Computation, 2015, 11, 3096-3103.	5.3	15
24	Nonsymmetrical perturbation theory for improving coupled-cluster wave functions. International Journal of Quantum Chemistry, 2002, 90, 1309-1320.	2.0	14
25	Idempotency-Conserving Iteration Scheme for the One-Electron Density Matrix. Physical Review Letters, 2005, 95, 013002.	7.8	14
26	Spin-adaptation and redundancy in state-specific multireference perturbation theory. Journal of Chemical Physics, 2013, 138, 124110.	3.0	14
27	Half-Projection of the Strongly Orthogonal Unrestricted Geminalsâ€™ Product Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 892-903.	5.3	14
28	Laplace-transformed denominators in perturbation theory: Linear-scaling second-order treatment of weakly interacting nanostructures. Physical Review A, 2003, 68, .	2.5	13
29	Spin Component Scaling in Multiconfiguration Perturbation Theory. Journal of Physical Chemistry A, 2011, 115, 523-534.	2.5	13
30	Role of triplet states in geminal-based perturbation theory. Molecular Physics, 2015, 113, 2960-2963.	1.7	13
31	Appendix to â€œStudies in Perturbation Theoryâ€: The Problem of Partitioning. , 2004, , 129-185.		13
32	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. International Journal of Quantum Chemistry, 1998, 70, 571-581.	2.0	12
33	Constant denominator perturbative schemes and the partitioning technique. International Journal of Quantum Chemistry, 2002, 90, 20-26.	2.0	12
34	Mayerâ€™s orthogonalization: relation to the Gram-Schmidt and LÃ¶wdinâ€™s symmetrical scheme. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	12
35	Multiple bond breaking with APSG-based correlation methods: comparison of two approaches. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12
36	Geminal perturbation theory based on the unrestricted Hartreeâ€“Fock wavefunction. Journal of Chemical Physics, 2019, 150, 034103.	3.0	10

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37	Dyson-corrected orbital energies for the perturbative treatment of electron correlation. International Journal of Quantum Chemistry, 1998, 69, 713-719.	2.0	9
38	Title is missing!. Structural Chemistry, 1999, 10, 149-155.	2.0	9
39	On the Use of Connected Moments Expansion with Coupled Cluster Reference. International Journal of Molecular Sciences, 2002, 3, 508-521.	4.1	9
40	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. Journal of Physical Chemistry A, 2016, 120, 5527-5538.	2.5	9
41	Convergence Enhancement in Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2004, 69, 105-120.	1.0	8
42	Unitary perturbation theory applied to multiconfigurational reference functions. International Journal of Quantum Chemistry, 2013, 113, 230-238.	2.0	8
43	Application of the Cauchy integral formula as a tool of analytic continuation for the resummation of divergent perturbation series. Journal of Chemical Physics, 2019, 150, 031101.	3.0	8
44	Optimized Quasiparticle Energies in Many-Body Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2003, 68, 331-339.	1.0	7
45	Novel orthogonalization and biorthogonalization algorithms. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
46	Size dependence of Feenberg scaling. International Journal of Quantum Chemistry, 2005, 101, 287-290.	2.0	6
47	Coupled-cluster theory and the method of moments. Computational and Theoretical Chemistry, 2006, 768, 17-23.	1.5	6
48	Frozen localized molecular orbitals in electron correlation calculations â€“ Exploiting the Hartreeâ€“Fock density matrix. Chemical Physics Letters, 2008, 450, 400-403.	2.6	6
49	Efficient iterative diagonalization of the Boseâ€“Hubbard model for ultracold bosons in a periodic optical trap. Chemical Physics, 2012, 401, 208-216.	1.9	6
50	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. Physica Status Solidi (B): Basic Research, 2014, 251, 2451-2456.	1.5	6
51	Effect of partitioning on the convergence properties of the Rayleigh-SchrÃ¶dinger perturbation series. Journal of Chemical Physics, 2017, 146, 124121.	3.0	6
52	The inverse boundary value problem: application in many-body perturbation theory. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
53	Ring coupled cluster doubles at the multireference level. Journal of Chemical Physics, 2020, 152, 204114.	3.0	6
54	Ring coupled-cluster doubles correction to geminal wavefunctions. Molecular Physics, 2017, 115, 2731-2742.	1.7	6

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55	Near-degeneracy corrections for second-order perturbation theory: comparison of two approaches. Theoretical Chemistry Accounts, 2001, 105, 408-412.	1.4	5
56	Multipartitioning MÃ¸llerâ€“Plesset perturbation theory: Sizeâ€extensivity at third order and symmetry conservation. International Journal of Quantum Chemistry, 2009, 109, 2554-2563.	2.0	5
57	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized Ï€-electron method. Journal of Chemical Physics, 2014, 140, 044112.	3.0	5
58	Energy error bars in direct configuration interaction iteration sequence. Journal of Chemical Physics, 2015, 143, 084112.	3.0	5
59	Improving half-projected spin-contaminated wave functions by multi-configuration perturbation theory. Journal of Chemical Physics, 2021, 154, 234110.	3.0	5
60	Calculation of correlation-corrected band structures of polymers in the case of quasi-degeneracy. Solid State Communications, 1997, 103, 639-644.	1.9	4
61	Optimized partitioning in PT: Application for the equation of motion describing ionization processes. International Journal of Quantum Chemistry, 2003, 92, 160-167.	2.0	4
62	Zero-field-splitting in triplet-state nanotubes. Chemical Physics Letters, 2010, 498, 292-295.	2.6	4
63	Symmetry-Adapted Perturbation with Half-Projection for Spin Unrestricted Geminals. Journal of Chemical Theory and Computation, 2021, 17, 4122-4143.	5.3	4
64	Fermi-Vacuum Invariance in Multiconfiguration Perturbation Theory. Progress in Theoretical Chemistry and Physics, 2009, , 257-268.	0.2	4
65	LÃ¶wdinâ€™s bracketing function revisited. Journal of Mathematical Chemistry, 2014, 52, 2210-2221.	1.5	3
66	Calculation of dispersion interactions with the geminal-based ring Coupled Cluster Doubles method. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
67	A Note on the Symmetry Properties of LÃ¶wdin's Orthogonalization Schemes. Collection of Czechoslovak Chemical Communications, 2008, 73, 937-944.	1.0	2
68	Perturbative Approximations to Avoid Matrix Diagonalization. Challenges and Advances in Computational Chemistry and Physics, 2011, , 83-95.	0.6	1
69	Dressing of Vertices by Cumulants in Multi-Reference Coupled Cluster. Journal of Chemical Theory and Computation, 2021, 17, 6947-6964.	5.3	1
70	On The Coupled-Cluster Equations. Stability Analysis And Nonstandard Correction Schemes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 513-534.	0.6	1
71	Stability analysis of the Lippmannâ€“Schwinger equation. Molecular Physics, 2023, 121, .	1.7	1
72	Preface to the special collection of theoretical chemistry accounts in honour of PÃ©ter R. SurjÃ¡n. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0

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73	On the variational principle for the non-linear SchrÃ¶dinger equation. Journal of Mathematical Chemistry, 2020, 58, 340-351.	1.5	0
74	Comment on â€œImproved many-body expansions from eigenvector continuationâ€• Physical Review C, 2021, 103, .	2.9	0
75	The $$gamma$$ function in quantum theory II. Mathematical challenges and paradoxa. Journal of Mathematical Chemistry, 2022, 60, 267-282.	1.5	0
76	Editorial: In memoriam IstvÃ¡n Mayer. International Journal of Quantum Chemistry, 2022, 122, .	2.0	0
77	A note on perturbation-adapted perturbation theory. Journal of Chemical Physics, 2022, 156, 116102.	3.0	0
78	Many-Body Perturbation Theory with Localized Orbitals: Accounting for Localization Diagrams as Integral Dressing. Journal of Chemical Theory and Computation, 2022, , .	5.3	0