Pu00e9ter G Szalay

List of Publications by Year
in descending order

127	9,326	47006 47	38395 95
papers	citations	h-index	g-index

132	132	132	4567
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691
2	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181.	47.7	559
3	Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI. Chemical Physics Letters, 1993, 214, 481-488.	2.6	427
4	High-level multireference methods in the quantum-chemistry program system COLUMBUS: Analytic MR-CISD and MR-AQCC gradients and MR-AQCC-LRT for excited states, GUGA spinâ€“orbit CI and parallel CI density. Physical Chemistry Chemical Physics, 2001, 3, 664-673.	2.8	401
5	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
6	A progress report on the status of the COLUMBUSMRCI program system. International Journal of Quantum Chemistry, 1988, 34, 149-165.	2.0	353
7	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. Journal of Chemical Physics, 2006, 125, 064108.	3.0	312
8	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. Journal of Chemical Physics, 2004, 120, 7322-7329.	3.0	290
9	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
10	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	4.2	283
11	A general state-selective multireference coupled-cluster algorithm. Journal of Chemical Physics, 2002, 117, 980-990.	3.0	237
12	Approximately extensive modifications of the multireference configuration interaction method: A theoretical and practical analysis. Journal of Chemical Physics, 1995, 103, 3600-3612.	3.0	225
13	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. Journal of Chemical Physics, 2004, 120, 7330-7339.	3.0	216
14	A general multireference configuration interaction gradient program. Journal of Chemical Physics, 1992, 96, 2085-2098.	3.0	205
15	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 144111.	3.0	182
16	Columbusâ€”a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199.	14.6	171
17	Analytic first derivatives for general coupled-cluster and configuration interaction models. Journal of Chemical Physics, 2003, 119, 2991-3004.	3.0	152
18	Decomposition modes of dioxirane, methyldioxirane and dimethyldioxirane â€” a CCSD(T), MR-AQCC and DFT investigation. Chemical Physics Letters, 1998, 292, 97-109.	2.6	129

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19	High-Level Electron Correlation Calculations on Formamide and the Resonance Model. Journal of Physical Chemistry A, 1997, 101, 1400-1408.	2.5	123
20	Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. Journal of Chemical Physics, 2002, 117, 2657-2671.	3.0	122
21	A systematic theoretical investigation of the valence excited states of the diatomic molecules B 2 , C 2 , N 2 and O 2. Theoretical Chemistry Accounts, 2001, 105, 227-243.	1.4	110
22	Benchmarking Coupled Cluster Methods on Valence Singlet Excited States. Journal of Chemical Theory and Computation, 2014, 10, 3757-3765.	5.3	109
23	Analytic energy derivatives for coupled-cluster methods describing excited states: General formulas and comparison of computational costs. International Journal of Quantum Chemistry, 1995, 55, 151-163.	2.0	103
24	Alternative ansÃtze in single reference coupledâ€cluster theory. III. A critical analysis of different methods. Journal of Chemical Physics, 1995, 103, 281-298.	3.0	103
25	Analytic UHF-CCSD(T) second derivatives: implementation and application to the calculation of the vibration-rotation interaction constants of NCO and NCS. Theoretical Chemistry Accounts, 1998, 100, 5-11.	1.4	103
26	New analytical model for the ozone electronic ground state potential surface and accurate ab initio vibrational predictions at high energy range. Journal of Chemical Physics, 2013, 139, 134307.	3.0	101
27	Multistate vibronic interactions in the benzene radical cation. I. Electronic structure calculations. Journal of Chemical Physics, 2002, 117, 2645-2656.	3.0	91
28	Benchmark Studies on the Building Blocks of DNA. 1. Superiority of Coupled Cluster Methods in Describing the Excited States of Nucleobases in the Franckâ€“Condon Region. Journal of Physical Chemistry A, 2012, 116, 6702-6710.	2.5	91
29	Tautomers of cytosine and their excited electronic states: a matrix isolation spectroscopic and quantum chemical study. Physical Chemistry Chemical Physics, 2011, 13, 6799.	2.8	82
30	Hilbert space multireference coupledâ€cluster methods. II. A model study on H8. Journal of Chemical Physics, 1992, 97, 4289-4300.	3.0	81
31	Spin-restricted open-shell coupled-cluster theory. Journal of Chemical Physics, 1997, 107, 9028-9038.	3.0	72
32	Spin-restricted open-shell coupled-cluster theory for excited states. Journal of Chemical Physics, 2000, 112, 4027-4036.	3.0	69
33	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. Physical Chemistry Chemical Physics, 2000, 2, 2067-2073.	2.8	68
34	Toward an Improved Ground State Potential Energy Surface of Ozone. Journal of Physical Chemistry A, 2010, 114, 9927-9935.	2.5	68
35	Stationary points on the S1 potential energy surface of C2H2. Journal of Chemical Physics, 1994, 101, 356-365.	3.0	67
36	Does the â€œReef Structureâ€•at the Ozone Transition State towards the Dissociation Exist? New Insight from Calculations and Ultrasensitive Spectroscopy Experiments. Physical Review Letters, 2014, 113, 143002.	7.8	66

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37	Analytic energy gradients for the twoâ€determinant coupled cluster method with application to singlet excited states of butadiene and ozone. Journal of Chemical Physics, 1994, 101, 4936-4944.	3.0	63
38	Benchmarking for Perturbative Triple-Excitations in EE-EOM-CC Methods. Journal of Physical Chemistry A, 2013, 117, 2569-2579.	2.5	63
39	Pathologic Alterations of the Outer Retina in Streptozotocin-Induced Diabetes. , 2014, 55, 3686.		62
40	New Versions of Approximately Extensive Corrected Multireference Configuration Interaction Methods. The Journal of Physical Chemistry, 1996, 100, 6288-6297.	2.9	59
41	Analytic evaluation of the nonadiabatic coupling vector between excited states using equation-of-motion coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 124104.	3.0	56
42	A systematic coupled-cluster investigation of structure and vibrational frequencies of the lowest electronic states of ketenyl radical. Chemical Physics Letters, 1992, 193, 573-579.	2.6	54
43	Accurate ab initio determination of the adiabatic potential energy function and the Bornâ€“Oppenheimer breakdown corrections for the electronic ground state of LiH isotopologues. Journal of Chemical Physics, 2011, 134, 094306.	3.0	54
44	SCF and electron correlation studies on structures and harmonic inâ€plane force fields of ethylene, trans 1,3â€butadiene, and allâ€trans 1,3,5â€hexatriene. Journal of Chemical Physics, 1987, 87, 3530-3538.	3.0	50
45	Perturbative treatment of the electron-correlation contribution to the diagonal Born-Oppenheimer correction. Journal of Chemical Physics, 2007, 127, 014102.	3.0	49
46	Accuracy of Coupled Cluster Excitation Energies in Diffuse Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 202-209.	5.3	49
47	High-quality theoretical potential energy surface for Be2 by using the multireference averaged quadratic coupled-cluster (MR-AQCC) method and large basis sets. Chemical Physics Letters, 1996, 258, 400-408.	2.6	48
48	A New Benchmark Set for Excitation Energy of Charge Transfer States: Systematic Investigation of Coupled Cluster Type Methods. Journal of Chemical Theory and Computation, 2020, 16, 4213-4225.	5.3	48
49	A new accurate ground-state potential energy surface of ethylene and predictions for rotational and vibrational energy levels. Journal of Chemical Physics, 2014, 141, 104301.	3.0	47
50	Towards a spin-adapted coupled-cluster theory for high-spin open-shell states. Journal of Chemical Physics, 2006, 124, 124105.	3.0	46
51	Geometry relaxation effects in the 1 1Bu and 2 1Ag states of trans-1,3-butadiene. Chemical Physics, 1989, 130, 219-228.	1.9	44
52	Anabinitiostudy of the structure and vibrational spectra of allyl and 1,4â€pentadienyl radicals. Journal of Chemical Physics, 1990, 93, 1246-1256.	3.0	44
53	The interaction between cytosine tautomers and water: an MP2 and coupled cluster electron correlation study. Chemical Physics Letters, 2002, 356, 383-390.	2.6	44
54	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. Journal of Chemical Physics, 2005, 122, 154107.	3.0	44

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55	Benchmark Thermochemistry of the Hydroperoxyl Radicalâ€. Journal of Physical Chemistry A, 2004, 108, 3195-3199.	2.5	43
56	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
57	Quantum chemical coupled cluster study of the structure and spectra of the ground and first excited states of the ketenyl radical. Chemical Physics Letters, 1996, 263, 91-99.	2.6	41
58	Equilibrium Geometry of the Ethynyl (CCH) Radicalâ€. Journal of Physical Chemistry A, 2004, 108, 3030-3034.	2.5	39
59	Triplet instability in doublet systems. Journal of Chemical Physics, 2004, 121, 7624.	3.0	38
60	Benchmark Studies on the Building Blocks of DNA. 3. Watsonâ€“Crick and Stacked Base Pairs. Journal of Physical Chemistry A, 2013, 117, 3149-3157.	2.5	37
61	Electronic states of ketene. Journal of Chemical Physics, 1996, 105, 1034-1045.	3.0	35
62	Vacuum Ultraviolet Spectroscopy of the Carbon Molecule C3 in Matrix Isolated State:â€‰ Experiment and Theory. Journal of Physical Chemistry A, 2002, 106, 5779-5788.	2.5	35
63	Benchmark Studies on the Building Blocks of DNA. 2. Effect of Biological Environment on the Electronic Excitation Spectrum of Nucleobases. Journal of Physical Chemistry A, 2012, 116, 8851-8860.	2.5	35
64	Theoretical prediction of the spin-orbit splitting in the NCO, NCS, HCCO and HCCS radicals. Journal of Chemical Physics, 1997, 106, 436-437.	3.0	34
65	Investigation of the Impact of Different Terms in the Second Order Hamiltonian on Excitation Energies of Valence and Rydberg States. Journal of Chemical Theory and Computation, 2016, 12, 5477-5482.	5.3	34
66	Ab initiodetermination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. Molecular Physics, 2005, 103, 2159-2168.	1.7	33
67	The Cl*f*â€‰2A2 excited state of NO2: Evidence for a Cs equilibrium structure and a failure of some spin-restricted reference wavefunctions. Journal of Chemical Physics, 1997, 107, 2525-2528.	3.0	32
68	Multi-mode vibronic interactions in the five lowest electronic states of the fluorobenzene radical cation. Chemical Physics, 2006, 329, 65-75.	1.9	31
69	The problem of interoperability: A common data format for quantum chemistry codes. International Journal of Quantum Chemistry, 2007, 107, 2082-2091.	2.0	31
70	Theoretical prediction of the electronic excited states and resonance Raman intensities in formamide from coupled cluster calculations. Chemical Physics Letters, 1997, 270, 406-412.	2.6	29
71	FORTRAN Interface for Code Interoperability in Quantum Chemistry:â€‰ The Q5Cost Library. Journal of Chemical Information and Modeling, 2007, 47, 1271-1277.	5.4	29
72	Reinterpretation of the UV Spectrum of Cytosine: Only Two Electronic Transitions?. ChemPhysChem, 2009, 10, 1603-1606.	2.1	29

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73	Accuracy of Spin-Component-Scaled CC2 Excitation Energies and Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 5523-5531.	5.3	28
74	The accuracy of molecular bond lengths computed by multireference electronic structure methods. Chemical Physics, 2008, 349, 37-57.	1.9	27
75	Relative stabilities of the s-cis and gauche structures of 1,3-butadiene. The Journal of Physical Chemistry, 1989, 93, 6629-6631.	2.9	26
76	Structure and spectra of the thioketenyl (HCCS) radical in its ground and first excited states obtained by ab initio coupledâ€cluster methods. Journal of Chemical Physics, 1996, 105, 2735-2743.	3.0	26
77	The enthalpy of formation of2II CH. Molecular Physics, 2002, 100, 3879-3883.	1.7	25
78	Benchmarking coupled cluster methods on singlet excited states of nucleobases. Journal of Molecular Modeling, 2014, 20, 2503.	1.8	25
79	Accurate 12D dipole moment surfaces of ethylene. Chemical Physics Letters, 2015, 639, 275-282.	2.6	25
80	Unimolecular Rearrangement oftrans-FONO to FNO2. A Possible Model System for Atmospheric Nitrate Formationâ€. Journal of Physical Chemistry A, 2004, 108, 7639-7642.	2.5	24
81	Multireference averaged quadratic coupled-cluster (MR-AQCC) method based on the functional of the total energy. Chemical Physics, 2008, 349, 121-125.	1.9	24
82	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	5.3	24
83	Accuracy of Spin-Component Scaled ADC(2) Excitation Energies and Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2020, 16, 468-474.	5.3	24
84	First-Principles Calculation of Electron Spin-Rotation Tensors. Journal of Physical Chemistry A, 2010, 114, 9246-9252.	2.5	23
85	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	3.3	22
86	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. Journal of Chemical Theory and Computation, 2014, 10, 1968-1979.	5.3	21
87	Are ab initio quantum chemistry methods able to predict vibrational states up to the dissociation limit for multi-electron molecules close to spectroscopic accuracy?. Physical Chemistry Chemical Physics, 2011, 13, 3654-3659.	2.8	19
88	TOWARDS STATE-SPECIFIC FORMULATION OF MULTIREFERENCE COUPLED-CLUSTER THEORY: COUPLED ELECTRON PAIR APPROXIMATIONS (CEPA) LEADING TO MULTIREFERENCE CONFIGURATION INTERACTION (MR-CI) TYPE EQUATIONS. Recent Advances in Computational, 1997, , 81-123.	0.8	18
89	Photodissociation of HOBr. I. Ab initio potential energy surfaces for the three lowest electronic states and calculation of rotationalâ€“vibrational energy levels and wave functions. Journal of Chemical Physics, 1999, 110, 8448-8460.	3.0	16
90	Spin-restricted coupled-cluster theory with triple excitations. Journal of Chemical Physics, 2002, 117, 7872-7881.	3.0	16

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91	Combined Jahnâ€“Teller and Pseudo-Jahnâ€“Teller Effects in the Benzene Radical Cation. Advances in Quantum Chemistry, 2003, 44, 199-217.	0.8	15
92	Diagonal Bornâ€“Oppenheimer corrections to the ground electronic state potential energy surfaces of ozone: improvement of ab initio vibrational band centers for the ¹⁶O₃, ¹⁷O₃ and ¹⁸O₃ isotopologues. Physical Chemistry Chemical Physics, 2020, 22, 24257-24269.	2.8	15
93	Coupled-Cluster Study of Spectroscopic Constants of the Alkali Metal Diatomics: Ground and the Singlet Excited States of Na2, NaLi, NaK, and NaRb. Collection of Czechoslovak Chemical Communications, 2005, 70, 951-978.	1.0	14
94	Improved Description of Charge-Transfer Potential Energy Surfaces via Spin-Component-Scaled CC2 and ADC(2) Methods. Journal of Chemical Theory and Computation, 2021, 17, 439-449.	5.3	14
95	Alternative ansï¿½tze in coupled-cluster theory. IV. Comparison for the two electron problem and the role of exclusion principle violating (EPV) terms. International Journal of Quantum Chemistry, 1992, 44, 85-106.	2.0	13
96	A priori results for molecular geometry, scaled quantum mechanical (SQM) force field, and vibrational spectra of pyridazine. The Journal of Physical Chemistry, 1993, 97, 1356-1363.	2.9	13
97	Theoretical study of the excitation spectrum of azomethane. Chemical Physics, 2011, 380, 9-16.	1.9	13
98	Details of the Excited-State Potential Energy Surfaces of Adenine by Coupled Cluster Techniques. Journal of Physical Chemistry A, 2014, 118, 6197-6207.	2.5	11
99	Quantum chemical MP2 results on some hydrates of cytosine: binding sites, energies and the first hydration shell. Physical Chemistry Chemical Physics, 2015, 17, 29880-29890.	2.8	11
100	Improving the Accuracy of the Charge Transfer Integrals Obtained by Coupled Cluster Theory, MBPT(2), and TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 5705-5711.	5.3	10
101	Characterization of the excited states of DNA building blocks: a coupled cluster computational study. Physical Chemistry Chemical Physics, 2016, 18, 23596-23606.	2.8	10
102	Geometry relaxation effects in the 1 1B2 and 2 1A1 states of cis-1,3-butadiene. Chemical Physics, 1990, 141, 355-363.	1.9	9
103	Comparison of sigma-point filters for state estimation of diabetes models. , 2014, , .		9
104	Fourier Transform Microwave Spectrum of Propene-3-d₁ (CH₂â•CHCH₂D), Quadrupole Coupling Constants of Deuterium, and a Semiexperimental Equilibrium Structure of Propene. Journal of Physical Chemistry A, 2017, 121, 3155-3166.	2.5	9
105	Potential energy surfaces of charge transfer states. Molecular Physics, 2020, 118, e1776903.	1.7	9
106	Can coupledâ€cluster methods be used to describe excited states of the building blocks of DNA?. International Journal of Quantum Chemistry, 2013, 113, 1821-1827.	2.0	8
107	Structure and Photoelectron Spectrum of Tetramethyldiarsane. Journal of the American Chemical Society, 1997, 119, 11926-11932.	13.7	6
108	Dimol Emission of Oxygen Made Possible by Repulsive Interaction. Journal of Physical Chemistry Letters, 2017, 8, 3356-3361.	4.6	5

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109	On our efforts constructing a proper multireference coupled-cluster method. Molecular Physics, 2010, 108, 3055-3065.	1.7	4
110	Quasi-Model-Based Control of Type 1 Diabetes Mellitus. Journal of Electrical and Computer Engineering, 2011, 2011, 1-12.	0.9	4
111	On the FCNSâ‡†FC(NS) reaction: A matrix isolation and theoretical study. Journal of Molecular Spectroscopy, 2015, 310, 8-15.	1.2	4
112	Development of highly accurate approximate scheme for computing the charge transfer integral. Journal of Chemical Physics, 2015, 143, 074109.	3.0	4
113	Comparison of approximate intermolecular potentials for ab initio fragment calculations on medium sized Nâ€heterocycles. Journal of Computational Chemistry, 2022, 43, 1079-1093.	3.3	3
114	Ab initio coupled-cluster study of 2II radicals in ground and excited states: application to NCO and NCS. Journal of Molecular Structure, 1997, 410-411, 305-309.	3.6	2
115	Efficient Sparse Matrix Algorithm to Speed Up the Calculation of the Ladder Term in Coupled Cluster Programs. Journal of Chemical Theory and Computation, 2012, 8, 3108-3118.	5.3	2
116	Long-term prediction for T1DM model during state-feedback control. , 2016, , .		2
117	First-principles interpretation of electron transport through single-molecule junctions using molecular dynamics of electron attached states. Molecular Physics, 2021, 119, .	1.7	2
118	Electron correlation and molecular dynamics for excited states and photochemistry. Chemical Physics, 2008, 349, vii-viii.	1.9	1
119	Model-based healthcare applications at Óbuda University. , 2014, , .		1
120	NMR and quantum chemical analysis of 3-(2-methly-2-phenylhydrazinyl)cyclohex-2-en-1-one. Journal of Molecular Modeling, 2014, 20, 2293.	1.8	1
121	Sensor Drift Compensation Using Fuzzy Interference System and Sparse-Grid Quadrature Filter in Blood Glucose Control. Lecture Notes in Computer Science, 2014, , 445-453.	1.3	1
122	Accurate calculations of ground and excited states by the MR-AQCC method. Prototype application to the proton transfer in 7-azaindol. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 457-467.	0.2	0
123	Uncertainties and Modeling Errors of Type 1 Diabetes Models. Lecture Notes in Bioengineering, 2016, , 211-225.	0.4	0
124	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
125	BevezetÅ‘. , 0, , 11-12.		0
126	Introduction to the John Stanton special issue. Molecular Physics, 0, , .	1.7	0

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127	Tunnelling lifetimes of the rovibronic levels in the B electronic state of the CH radical obtained from ab initio data. Molecular Physics, 1999, 96, 359-366.	1.7	0