

Pu00e9ter G Szalay

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8083849/publications.pdf>

Version: 2024-02-01

127
papers

9,326
citations

47006

47
h-index

38395

95
g-index

132
all docs

132
docs citations

132
times ranked

4567
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparison of approximate intermolecular potentials for ab initio fragment calculations on medium sized N-heterocycles. Journal of Computational Chemistry, 2022, 43, 1079-1093.	3.3	3
2	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
3	First-principles interpretation of electron transport through single-molecule junctions using molecular dynamics of electron attached states. Molecular Physics, 2021, 119, .	1.7	2
4	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
5	Diagonal Born-Oppenheimer corrections to the ground electronic state potential energy surfaces of ozone: improvement of <i>ab initio</i> vibrational band centers for the ¹⁶ O ₃ , ¹⁷ O ₃ and ¹⁸ O ₃ isotopologues. Physical Chemistry Chemical Physics, 2020, 22, 24257-24269.	2.8	15
6	Potential energy surfaces of charge transfer states. Molecular Physics, 2020, 118, e1776903.	1.7	9
7	Coupled-cluster techniques for computational chemistry: The <code>CFOUR</code> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
8	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
9	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
10	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
11	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	5.3	24
12	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
13	Fourier Transform Microwave Spectrum of Propene-3- <i>d</i> ₁ (CH ₂ -CHCH ₂ D), Quadrupole Coupling Constants of Deuterium, and a Semiexperimental Equilibrium Structure of Propene. Journal of Physical Chemistry A, 2017, 121, 3155-3166.	2.5	9
14	Accuracy of Coupled Cluster Excitation Energies in Diffuse Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 202-209.	5.3	49
15	Dimol Emission of Oxygen Made Possible by Repulsive Interaction. Journal of Physical Chemistry Letters, 2017, 8, 3356-3361.	4.6	5
16	Long-term prediction for T1DM model during state-feedback control. , 2016, , .		2
17	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
18	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

#	ARTICLE	IF	CITATIONS
19	Uncertainties and Modeling Errors of Type 1 Diabetes Models. Lecture Notes in Bioengineering, 2016, , 211-225.	0.4	0
20	Preface to the special collection of theoretical chemistry accounts in honour of P�ter R. Surj�n. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0
21	On the FCNS�FC(NS) reaction: A matrix isolation and theoretical study. Journal of Molecular Spectroscopy, 2015, 310, 8-15.	1.2	4
22	Accurate 12D dipole moment surfaces of ethylene. Chemical Physics Letters, 2015, 639, 275-282.	2.6	25
23	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
24	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
25	Development of highly accurate approximate scheme for computing the charge transfer integral. Journal of Chemical Physics, 2015, 143, 074109.	3.0	4
26	Benchmarking coupled cluster methods on singlet excited states of nucleobases. Journal of Molecular Modeling, 2014, 20, 2503.	1.8	25
27	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
28	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
29	Does the "Reef Structure" 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
30	Model-based healthcare applications at �buda University. , 2014, , .		1
31	Comparison of sigma-point filters for state estimation of diabetes models. , 2014, , .		9
32	Benchmarking Coupled Cluster Methods on Valence Singlet Excited States. Journal of Chemical Theory and Computation, 2014, 10, 3757-3765.	5.3	109
33	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
34	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
35	Pathologic Alterations of the Outer Retina in Streptozotocin-Induced Diabetes. , 2014, 55, 3686.		62
36	NMR and quantum chemical analysis of 3-(2-methyl-2-phenylhydrazinyl)cyclohex-2-en-1-one. Journal of Molecular Modeling, 2014, 20, 2293.	1.8	1

#	ARTICLE	IF	CITATIONS
37	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
38	Benchmarking for Perturbative Triple-Excitations in EE-EOM-CC Methods. Journal of Physical Chemistry A, 2013, 117, 2569-2579.	2.5	63
39	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
40	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
41	New analytical model for the ozone electronic ground state potential surface and accurate <i>ab initio</i> vibrational predictions at high energy range. Journal of Chemical Physics, 2013, 139, 134307.	3.0	101
42	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181.	47.7	559
43	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
44	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
45	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
46	Accurate <i>ab initio</i> 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
47	Are <i>ab initio</i> 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
48	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
49	Columbusâ€™a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199.	14.6	171
50	Theoretical study of the excitation spectrum of azomethane. Chemical Physics, 2011, 380, 9-16.	1.9	13
51	Quasi-Model-Based Control of Type 1 Diabetes Mellitus. Journal of Electrical and Computer Engineering, 2011, 2011, 1-12.	0.9	4
52	Toward an Improved Ground State Potential Energy Surface of Ozone. Journal of Physical Chemistry A, 2010, 114, 9927-9935.	2.5	68
53	On our efforts constructing a proper multireference coupled-cluster method. Molecular Physics, 2010, 108, 3055-3065.	1.7	4
54	First-Principles Calculation of Electron Spin-Rotation Tensors. Journal of Physical Chemistry A, 2010, 114, 9246-9252.	2.5	23

#	ARTICLE	IF	CITATIONS
55	Reinterpretation of the UV Spectrum of Cytosine: Only Two Electronic Transitions?. <i>ChemPhysChem</i> , 2009, 10, 1603-1606.	2.1	29
56	Analytic evaluation of the nonadiabatic coupling vector between excited states using equation-of-motion coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2009, 131, 124104.	3.0	56
57	Electron correlation and molecular dynamics for excited states and photochemistry. <i>Chemical Physics</i> , 2008, 349, vii-viii.	1.9	1
58	The accuracy of molecular bond lengths computed by multireference electronic structure methods. <i>Chemical Physics</i> , 2008, 349, 37-57.	1.9	27
59	Multireference averaged quadratic coupled-cluster (MR-AQCC) method based on the functional of the total energy. <i>Chemical Physics</i> , 2008, 349, 121-125.	1.9	24
60	FORTTRAN Interface for Code Interoperability in Quantum Chemistry: The Q5Cost Library. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1271-1277.	5.4	29
61	Perturbative treatment of the electron-correlation contribution to the diagonal Born-Oppenheimer correction. <i>Journal of Chemical Physics</i> , 2007, 127, 014102.	3.0	49
62	The problem of interoperability: A common data format for quantum chemistry codes. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2082-2091.	2.0	31
63	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. <i>Journal of Chemical Physics</i> , 2006, 125, 064108.	3.0	312
64	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2006, 125, 144111.	3.0	182
65	Towards a spin-adapted coupled-cluster theory for high-spin open-shell states. <i>Journal of Chemical Physics</i> , 2006, 124, 124105.	3.0	46
66	Multi-mode vibronic interactions in the five lowest electronic states of the fluorobenzene radical cation. <i>Chemical Physics</i> , 2006, 329, 65-75.	1.9	31
67	Coupled-Cluster Study of Spectroscopic Constants of the Alkali Metal Diatomics: Ground and the Singlet Excited States of Na ₂ , NaLi, NaK, and NaRb. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 951-978.	1.0	14
68	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. <i>Journal of Chemical Physics</i> , 2005, 122, 154107.	3.0	44
69	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. <i>Journal of Physical and Chemical Reference Data</i> , 2005, 34, 573-656.	4.2	283
70	Ab initiodetermination of the heat of formation of ketyl (HCCO) and ethynyl (CCH) radicals. <i>Molecular Physics</i> , 2005, 103, 2159-2168.	1.7	33
71	HEAT: High accuracy extrapolated ab initio thermochemistry. <i>Journal of Chemical Physics</i> , 2004, 121, 11599-11613.	3.0	691
72	Triplet instability in doublet systems. <i>Journal of Chemical Physics</i> , 2004, 121, 7624.	3.0	38

#	ARTICLE	IF	CITATIONS
73	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. <i>Journal of Chemical Physics</i> , 2004, 120, 7330-7339.	3.0	216
74	Benchmark Thermochemistry of the Hydroperoxyl Radical. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3195-3199.	2.5	43
75	Equilibrium Geometry of the Ethynyl (CCH) Radical. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3030-3034.	2.5	39
76	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. <i>Journal of Chemical Physics</i> , 2004, 120, 7322-7329.	3.0	290
77	Unimolecular Rearrangement of trans-FONO to FNO ₂ . A Possible Model System for Atmospheric Nitrate Formation. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7639-7642.	2.5	24
78	Analytic first derivatives for general coupled-cluster and configuration interaction models. <i>Journal of Chemical Physics</i> , 2003, 119, 2991-3004.	3.0	152
79	Combined Jahn-Teller and Pseudo-Jahn-Teller Effects in the Benzene Radical Cation. <i>Advances in Quantum Chemistry</i> , 2003, 44, 199-217.	0.8	15
80	The enthalpy of formation of 2H ₂ CH. <i>Molecular Physics</i> , 2002, 100, 3879-3883.	1.7	25
81	Spin-restricted coupled-cluster theory with triple excitations. <i>Journal of Chemical Physics</i> , 2002, 117, 7872-7881.	3.0	16
82	Vacuum Ultraviolet Spectroscopy of the Carbon Molecule C ₃ in Matrix Isolated State: Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5779-5788.	2.5	35
83	Multistate vibronic interactions in the benzene radical cation. I. Electronic structure calculations. <i>Journal of Chemical Physics</i> , 2002, 117, 2645-2656.	3.0	91
84	Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. <i>Journal of Chemical Physics</i> , 2002, 117, 2657-2671.	3.0	122
85	A general state-selective multireference coupled-cluster algorithm. <i>Journal of Chemical Physics</i> , 2002, 117, 980-990.	3.0	237
86	Accurate calculations of ground and excited states by the MR-AQCC method. Prototype application to the proton transfer in 7-azaindol. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2002, 2, 457-467.	0.2	0
87	The interaction between cytosine tautomers and water: an MP2 and coupled cluster electron correlation study. <i>Chemical Physics Letters</i> , 2002, 356, 383-390.	2.6	44
88	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 spin-orbit CI and parallel CI density. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 664-673.	2.8	401
89	A systematic theoretical investigation of the valence excited states of the diatomic molecules B ₂ , C ₂ , N ₂ and O ₂ . <i>Theoretical Chemistry Accounts</i> , 2001, 105, 227-243.	1.4	110
90	Spin-restricted open-shell coupled-cluster theory for excited states. <i>Journal of Chemical Physics</i> , 2000, 112, 4027-4036.	3.0	69

#	ARTICLE	IF	CITATIONS
91	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2067-2073.	2.8	68
92	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. <i>Journal of Chemical Physics</i> , 1999, 110, 8448-8460.	3.0	16
93	Tunnelling lifetimes of the rovibronic levels in the B electronic state of the CH radical obtained from ab initio data. <i>Molecular Physics</i> , 1999, 96, 359-366.	1.7	0
94	Decomposition modes of dioxirane, methyldioxirane and dimethyldioxirane â€” a CCSD(T), MR-AQCC and DFT investigation. <i>Chemical Physics Letters</i> , 1998, 292, 97-109.	2.6	129
95	Analytic UHF-CCSD(T) second derivatives: implementation and application to the calculation of the vibration-rotation interaction constants of NCO and NCS. <i>Theoretical Chemistry Accounts</i> , 1998, 100, 5-11.	1.4	103
96	Theoretical prediction of the spin-orbit splitting in the NCO, NCS, HCCO and HCCS radicals. <i>Journal of Chemical Physics</i> , 1997, 106, 436-437.	3.0	34
97	The C ₁ â€“A ₂ excited state of NO ₂ : Evidence for a Cs equilibrium structure and a failure of some spin-restricted reference wavefunctions. <i>Journal of Chemical Physics</i> , 1997, 107, 2525-2528.	3.0	32
98	Spin-restricted open-shell coupled-cluster theory. <i>Journal of Chemical Physics</i> , 1997, 107, 9028-9038.	3.0	72
99	Structure and Photoelectron Spectrum of Tetramethyldiarsane. <i>Journal of the American Chemical Society</i> , 1997, 119, 11926-11932.	13.7	6
100	TOWARDS STATE-SPECIFIC FORMULATION OF MULTIREFERENCE COUPLED-CLUSTER THEORY: COUPLED ELECTRON PAIR APPROXIMATIONS (CEPA) LEADING TO MULTIREFERENCE CONFIGURATION INTERACTION (MR-CI) TYPE EQUATIONS. <i>Recent Advances in Computational</i> , 1997, , 81-123.	0.8	18
101	High-Level Electron Correlation Calculations on Formamide and the Resonance Model. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1400-1408.	2.5	123
102	Ab initio coupled-cluster study of 2II radicals in ground and excited states: application to NCO and NCS. <i>Journal of Molecular Structure</i> , 1997, 410-411, 305-309.	3.6	2
103	Theoretical prediction of the electronic excited states and resonance Raman intensities in formamide from coupled cluster calculations. <i>Chemical Physics Letters</i> , 1997, 270, 406-412.	2.6	29
104	High-quality theoretical potential energy surface for Be ₂ by using the multireference averaged quadratic coupled-cluster (MR-AQCC) method and large basis sets. <i>Chemical Physics Letters</i> , 1996, 258, 400-408.	2.6	48
105	Quantum chemical coupled cluster study of the structure and spectra of the ground and first excited states of the ketyenyl radical. <i>Chemical Physics Letters</i> , 1996, 263, 91-99.	2.6	41
106	Structure and spectra of the thioketyenyl (HCCS) radical in its ground and first excited states obtained by ab initio coupledâ€“cluster methods. <i>Journal of Chemical Physics</i> , 1996, 105, 2735-2743.	3.0	26
107	Electronic states of ketene. <i>Journal of Chemical Physics</i> , 1996, 105, 1034-1045.	3.0	35
108	New Versions of Approximately Extensive Corrected Multireference Configuration Interaction Methods. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6288-6297.	2.9	59

#	ARTICLE	IF	CITATIONS
109	Analytic energy derivatives for coupled-cluster methods describing excited states: General formulas and comparison of computational costs. <i>International Journal of Quantum Chemistry</i> , 1995, 55, 151-163.	2.0	103
110	Approximately extensive modifications of the multireference configuration interaction method: A theoretical and practical analysis. <i>Journal of Chemical Physics</i> , 1995, 103, 3600-3612.	3.0	225
111	Alternative ansätze in single reference coupled-cluster theory. III. A critical analysis of different methods. <i>Journal of Chemical Physics</i> , 1995, 103, 281-298.	3.0	103
112	Stationary points on the S1 potential energy surface of C2H2. <i>Journal of Chemical Physics</i> , 1994, 101, 356-365.	3.0	67
113	Analytic energy gradients for the two-determinant coupled cluster method with application to singlet excited states of butadiene and ozone. <i>Journal of Chemical Physics</i> , 1994, 101, 4936-4944.	3.0	63
114	Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI. <i>Chemical Physics Letters</i> , 1993, 214, 481-488.	2.6	427
115	A priori results for molecular geometry, scaled quantum mechanical (SQM) force field, and vibrational spectra of pyridazine. <i>The Journal of Physical Chemistry</i> , 1993, 97, 1356-1363.	2.9	13
116	A general multireference configuration interaction gradient program. <i>Journal of Chemical Physics</i> , 1992, 96, 2085-2098.	3.0	205
117	Hilbert space multireference coupled-cluster methods. II. A model study on H8. <i>Journal of Chemical Physics</i> , 1992, 97, 4289-4300.	3.0	81
118	Alternative ansätze in coupled-cluster theory. IV. Comparison for the two electron problem and the role of exclusion principle violating (EPV) terms. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 85-106.	2.0	13
119	A systematic coupled-cluster investigation of structure and vibrational frequencies of the lowest electronic states of ketyl radical. <i>Chemical Physics Letters</i> , 1992, 193, 573-579.	2.6	54
120	Geometry relaxation effects in the 1 B2 and 2 1A1 states of cis-1,3-butadiene. <i>Chemical Physics</i> , 1990, 141, 355-363.	1.9	9
121	An ab initio study of the structure and vibrational spectra of allyl and 1,4-pentadienyl radicals. <i>Journal of Chemical Physics</i> , 1990, 93, 1246-1256.	3.0	44
122	Relative stabilities of the s-cis and gauche structures of 1,3-butadiene. <i>The Journal of Physical Chemistry</i> , 1989, 93, 6629-6631.	2.9	26
123	Geometry relaxation effects in the 1 B _u and 2 1A _g states of trans-1,3-butadiene. <i>Chemical Physics</i> , 1989, 130, 219-228.	1.9	44
124	A progress report on the status of the COLUMBUSMRCI program system. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 149-165.	2.0	353
125	SCF and electron correlation studies on structures and harmonic in-plane force fields of ethylene, trans-1,3-butadiene, and all-trans-1,3,5-hexatriene. <i>Journal of Chemical Physics</i> , 1987, 87, 3530-3538.	3.0	50
126	Bevezet, 0, , 11-12.		0

#	ARTICLE	IF	CITATIONS
127	Introduction to the John Stanton special issue. Molecular Physics, 0, , .	1.7	0