P u00e9ter G Szalay

List of Publications by Citations

121 papers	8,130 citations	45 h-index	89 g-index
131 ext. papers	8,699 ext. citations	4.6 avg, IF	5.94 L-index

#	Paper	IF	Citations
121	HEAT: High accuracy extrapolated ab initio thermochemistry. *Journal of Chemical Physics*, **2004**, 121, 11599-613	3.9	606
120	Multiconfiguration self-consistent field and multireference configuration interaction methods and applications. *Chemical Reviews*, **2012**, 112, 108-81	68.1	462
119	Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI. *Chemical Physics Letters*, **1993**, 214, 481-488	2.5	386
118	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. *Physical Chemistry Chemical Physics*, **2001**, 3, 664-673	3.6	369
117	A progress report on the status of the COLUMBUS MRCI program system. *International Journal of Quantum Chemistry*, **1988**, 34, 149-165	2.1	343
116	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. *Journal of Chemical Physics*, **2006**, 125, 64108	3.9	277
115	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. *Journal of Physical and Chemical Reference Data*, **2005**, 34, 573-656	4.3	275
114	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. *Journal of Chemical Physics*, **2004**, 120, 7322-9	3.9	270
113	A general state-selective multireference coupled-cluster algorithm. *Journal of Chemical Physics*, **2002**, 117, 980-990	3.9	227
112	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, 7330-9	3.9	208
111	Approximately extensive modifications of the multireference configuration interaction method: A theoretical and practical analysis. *Journal of Chemical Physics*, **1995**, 103, 3600-3612	3.9	205
110	A general multireference configuration interaction gradient program. *Journal of Chemical Physics*, **1992**, 96, 2085-2098	3.9	198
109	Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361	68.1	181
108	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. *Journal of Chemical Physics*, **2006**, 125, 144111	3.9	164
107	Coupled-cluster techniques for computational chemistry: The CFOUR program package. *Journal of Chemical Physics*, **2020**, 152, 214108	3.9	156
106	Columbus□ program system for advanced multireference theory calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 191-199	7.9	147
105	Analytic first derivatives for general coupled-cluster and configuration interaction models. *Journal of Chemical Physics*, **2003**, 119, 2991-3004	3.9	138

104	Decomposition modes of dioxirane, methyldioxirane and dimethyldioxirane a CCSD(T), MR-AQCC and DFT investigation. *Chemical Physics Letters*, **1998**, 292, 97-109	2.5	121
103	High-Level Electron Correlation Calculations on Formamide and the Resonance Model. *Journal of Physical Chemistry A*, **1997**, 101, 1400-1408	2.8	118
102	Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. *Journal of Chemical Physics*, **2002**, 117, 2657-2671	3.9	114
101	A systematic theoretical investigation of the valence excited states of the diatomic molecules B2, C2, N2 and O2. *Theoretical Chemistry Accounts*, **2001**, 105, 227-243	1.9	102
100	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	2.1	101
99	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	1.9	97
98	Benchmarking Coupled Cluster Methods on Valence Singlet Excited States. *Journal of Chemical Theory and Computation*, **2014**, 10, 3757-65	6.4	94
97	Alternative ansze in single reference coupled-cluster theory. III. A critical analysis of different methods. *Journal of Chemical Physics*, **1995**, 103, 281-298	3.9	90
96	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	3.9	88
95	Multistate vibronic interactions in the benzene radical cation. I. Electronic structure calculations. *Journal of Chemical Physics*, **2002**, 117, 2645-2656	3.9	85
94	Benchmark studies on the building blocks of DNA. 1. Superiority of coupled cluster methods in describing the excited states of nucleobases in the Franck-Condon region. *Journal of Physical Chemistry A*, **2012**, 116, 6702-10	2.8	80
93	Hilbert space multireference coupled-cluster methods. II. A model study on H8. *Journal of Chemical Physics*, **1992**, 97, 4289-4300	3.9	79
92	Tautomers of cytosine and their excited electronic states: a matrix isolation spectroscopic and quantum chemical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 6799-807	3.6	73
91	Spin-restricted open-shell coupled-cluster theory for excited states. *Journal of Chemical Physics*, **2000**, 112, 4027-4036	3.9	67
90	Spin-restricted open-shell coupled-cluster theory. *Journal of Chemical Physics*, **1997**, 107, 9028-9038	3.9	66
89	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	7.4	61
88	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. *Physical Chemistry Chemical Physics*, **2000**, 2, 2067-2073	3.6	61
87	Stationary points on the S1 potential energy surface of C2H2. *Journal of Chemical Physics*, **1994**, 101, 356-365	3.9	61

86	Toward an improved ground state potential energy surface of ozone. *Journal of Physical Chemistry A*, **2010**, 114, 9927-35	2.8	58
85	New Versions of Approximately Extensive Corrected Multireference Configuration Interaction Methods *The Journal of Physical Chemistry*, **1996**, 100, 6288-6297		58
84	Analytic energy gradients for the two-determinant coupled cluster method with application to singlet excited states of butadiene and ozone. *Journal of Chemical Physics*, **1994**, 101, 4936-4944	3.9	53
83	Benchmarking for perturbative triple-excitations in EE-EOM-CC methods. *Journal of Physical Chemistry A*, **2013**, 117, 2569-79	2.8	51
82	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	2.5	51
81	Analytic evaluation of the nonadiabatic coupling vector between excited states using equation-of-motion coupled-cluster theory. *Journal of Chemical Physics*, **2009**, 131, 124104	3.9	49
80	Accurate ab initio determination of the adiabatic potential energy function and the Born-Oppenheimer breakdown corrections for the electronic ground state of LiH isotopologues. *Journal of Chemical Physics*, **2011**, 134, 094306	3.9	48
79	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. *Journal of Chemical Physics*, **1987**, 87, 3530-3538	3.9	48
78	Pathologic alterations of the outer retina in streptozotocin-induced diabetes **2014**, 55, 3686-99		46
77	Towards a spin-adapted coupled-cluster theory for high-spin open-shell states. *Journal of Chemical Physics*, **2006**, 124, 124105	3.9	45
76	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	2.5	45
75	Perturbative treatment of the electron-correlation contribution to the diagonal Born-Oppenheimer correction. *Journal of Chemical Physics*, **2007**, 127, 014102	3.9	44
74	The interaction between cytosine tautomers and water: an MP2 and coupled cluster electron correlation study. *Chemical Physics Letters*, **2002**, 356, 383-390	2.5	42
73	Geometry relaxation effects in the 1 1Bu and 2 1Ag states of trans-1,3-butadiene. *Chemical Physics*, **1989**, 130, 219-228	2.3	42
72	An ab initio study of the structure and vibrational spectra of allyl and 1,4-pentadienyl radicals. *Journal of Chemical Physics*, **1990**, 93, 1246-1256	3.9	42
71	Benchmark Thermochemistry of the Hydroperoxyl Radical *Journal of Physical Chemistry A*, **2004**, 108, 3195-3199	2.8	41
70	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	2.5	40
69	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	3.9	39

68	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. *Journal of Chemical Physics*, **2005**, 122, 154107	3.9	39
67	Accuracy of Coupled Cluster Excitation Energies in Diffuse Basis Sets. *Journal of Chemical Theory and Computation*, **2017**, 13, 202-209	6.4	37
66	Triplet instability in doublet systems. *Journal of Chemical Physics*, **2004**, 121, 7624-31	3.9	37
65	Equilibrium Geometry of the Ethynyl (CCH) Radical *Journal of Physical Chemistry A*, **2004**, 108, 3030-3034	2.8	36
64	Benchmark studies on the building blocks of DNA. 3. Watson-Crick and stacked base pairs. *Journal of Physical Chemistry A*, **2013**, 117, 3149-57	2.8	35
63	Vacuum Ultraviolet Spectroscopy of the Carbon Molecule C3 in Matrix Isolated State: Experiment and Theory. *Journal of Physical Chemistry A*, **2002**, 106, 5779-5788	2.8	35
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55	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	6.4	27
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53	The accuracy of molecular bond lengths computed by multireference electronic structure methods. *Chemical Physics*, **2008**, 349, 37-57	2.3	27
52	FORTRAN interface for code interoperability in quantum chemistry: the Q5Cost library. *Journal of Chemical Information and Modeling*, **2007**, 47, 1271-7	6.1	26
51	Structure and spectra of the thioketenyl (HCCS) radical in its ground and first excited states obtained by ab initio coupled-cluster methods. *Journal of Chemical Physics*, **1996**, 105, 2735-2743	3.9	26

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49	Theoretical prediction of the electronic excited states and resonance Raman intensities in formamide from coupled cluster calculations. *Chemical Physics Letters*, **1997**, 270, 406-412	2.5	25
48	Unimolecular Rearrangement of trans-FONO to FNO2. A Possible Model System for Atmospheric Nitrate Formation *Journal of Physical Chemistry A*, **2004**, 108, 7639-7642	2.8	24
47	The enthalpy of formation of 2II CH. *Molecular Physics*, **2002**, 100, 3879-3883	1.7	24
46	Accurate 12D dipole moment surfaces of ethylene. *Chemical Physics Letters*, **2015**, 639, 275-282	2.5	22
45	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
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43	Benchmarking coupled cluster methods on singlet excited states of nucleobases. *Journal of Molecular Modeling*, **2014**, 20, 2503	2	21
42	Relative stabilities of the s-cis and gauche structures of 1,3-butadiene. *The Journal of Physical Chemistry*, **1989**, 93, 6629-6631		21
41	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2014**, 10, 1968-79	6.4	19
40	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2018**, 14, 5859-5869	6.4	19
39	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, 3654-9	3.6	18
38	First-principles calculation of electron spin-rotation tensors. *Journal of Physical Chemistry A*, **2010**, 114, 9246-52	2.8	18
37	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, **2014**, 35, 611-21	3.5	17
36	Accuracy of Spin-Component-Scaled CC2 Excitation Energies and Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2019**, 15, 5523-5531	6.4	16
35	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		16
34	Spin-restricted coupled-cluster theory with triple excitations. *Journal of Chemical Physics*, **2002**, 117, 7872-7881	3.9	16
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32	Theoretical study of the excitation spectrum of azomethane. *Chemical Physics*, **2011**, 380, 9-16	2.3	13
31	Alternative ansätze 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	2.1	13
30	Accuracy of Spin-Component Scaled ADC(2) Excitation Energies and Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2020**, 16, 468-474	6.4	13
29	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		12
28	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		12
27	Details of the excited-state potential energy surfaces of adenine by coupled cluster techniques. *Journal of Physical Chemistry A*, **2014**, 118, 6197-207	2.8	11
26	Photodissociation of HOBr. I. Ab initio potential energy surfaces for the three lowest electronic states and calculation of rotational–vibrational energy levels and wave functions. *Journal of Chemical Physics*, **1999**, 110, 8448-8460	3.9	11
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24	Can coupled-cluster methods be used to describe excited states of the building blocks of DNA?. *International Journal of Quantum Chemistry*, **2013**, 113, 1821-1827	2.1	8
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21	Configuration Interaction: Corrections for Size-Consistency		8
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19	Fourier Transform Microwave Spectrum of Propene-3-d (CH?CHCHD), Quadrupole Coupling Constants of Deuterium, and a Semiexperimental Equilibrium Structure of Propene. *Journal of Physical Chemistry A*, **2017**, 121, 3155-3166	2.8	6
18	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, 5705-11	6.4	6
17	Comparison of sigma-point filters for state estimation of diabetes models **2014**,		6
16	Structure and Photoelectron Spectrum of Tetramethyldiarsane. *Journal of the American Chemical Society*, **1997**, 119, 11926-11932	16.4	6
15	On the FCNS?FC(NS) reaction: A matrix isolation and theoretical study. *Journal of Molecular Spectroscopy*, **2015**, 310, 8-15	1.3	4

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13	Potential energy surfaces of charge transfer states. *Molecular Physics*, **2020**, 118, e1776903	1.7	4
12	Dimol Emission of Oxygen Made Possible by Repulsive Interaction. *Journal of Physical Chemistry Letters*, **2017**, 8, 3356-3361	6.4	4
11	On our efforts constructing a proper multireference coupled-cluster method. *Molecular Physics*, **2010**, 108, 3055-3065	1.7	3
10	Long-term prediction for T1DM model during state-feedback control **2016**,		2
9	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, 3108-18	6.4	2
8	Quasi-Model-Based Control of Type 1 Diabetes Mellitus. *Journal of Electrical and Computer Engineering*, **2011**, 2011, 1-12	1.9	2
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6	NMR and quantum chemical analysis of 3-(2-methly-2-phenylhydrazinyl)cyclohex-2-en-1-one. *Journal of Molecular Modeling*, **2014**, 20, 2293	2	1
5	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	3.4	1
4	Uncertainties and Modeling Errors of Type 1 Diabetes Models. *Lecture Notes in Bioengineering*, **2016** , 211-225	0.8	
3	Preface to the special collection of theoretical chemistry accounts in honour of PEer R. Surjn. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	
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1	Sensor Drift Compensation Using Fuzzy Interference System and Sparse-Grid Quadrature Filter in Blood Glucose Control. *Lecture Notes in Computer Science*, **2014**, 445-453	0.9	