GÃ¡bor CzakÃ³

List of Publications by Year
in descending order

110 papers	4,729 citations	81839 39 h-index	106281 65 g-index
110 all docs	110 docs citations	110 times ranked	1892 citing authors

#	Article	IF	Citations
1	Benchmark ab initio proton affinity and gasâ€phase basicity of Î±â€alanine based on coupledâ€cluster theory and statistical mechanics. Journal of Computational Chemistry, 2022, 43, 19-28.	1.5	4
2	ManyHF: A pragmatic automated method of finding lower-energy Hartreeâ€“Fock solutions for potential energy surface development. Journal of Chemical Physics, 2022, 156, 071101.	1.2	11
3	S_N2 Reactions with an Ambident Nucleophile: A Benchmark Ab Initio Study of the CN^{â€“} + CH₃Y [Y = F, Cl, Br, and I] Systems. Journal of Physical Chemistry A, 2022, 126, 889-900.	1.1	7
4	Vibrational mode-specific dynamics of the F^{â˜} + CH₃CH₂Cl multi-channel reaction. Physical Chemistry Chemical Physics, 2022, 24, 8166-8181.	1.3	12
5	Rotational Mode-Specificity in the Cl + C₂H₆ â†' HCl + C₂H₅ Reaction. Journal of Physical Chemistry A, 2022, 126, 2551-2560.	1.1	4
6	Unconventional SN2 retention pathways induced by complex formation: High-level dynamics investigation of the NH2â˜ + CH3I polyatomic reaction. Journal of Chemical Physics, 2022, 156, 184306.	1.2	6
7	Benchmark Ab Initio Characterization of the Abstraction and Substitution Pathways of the Cl + CH₃CN Reaction. Journal of Physical Chemistry A, 2022, 126, 2802-2810.	1.1	2
8	Benchmark ab initio stationary-point characterization of the complex potential energy surface of the multi-channel Cl + CH₃NH₂ reaction. Physical Chemistry Chemical Physics, 2021, 23, 10347-10356.	1.3	7
9	Facilitated inversion complicates the stereodynamics of an S_N2 reaction at nitrogen center. Chemical Science, 2021, 12, 5410-5418.	3.7	14
10	Benchmark ab initio proton affinity of glycine. Physical Chemistry Chemical Physics, 2021, 23, 9663-9671.	1.3	9
11	A benchmark ab initio study of the complex potential energy surfaces of the OH^{â˜} + CH₃CH₂Y [Y = F, Cl, Br, I] reactions. Physical Chemistry Chemical Physics, 2021, 23, 13526-13534.	1.3	7
12	First-Principles Reaction Dynamics beyond Six-Atom Systems. Journal of Physical Chemistry A, 2021, 125, 2385-2393.	1.1	14
13	Atomistic dynamics of elimination and nucleophilic substitution disentangled for the Fâ˜â€‰+â€‰CH3CH2Cl reaction. Nature Chemistry, 2021, 13, 977-981.	6.6	43
14	Detailed quasiclassical dynamics of the Fâ˜ + CH3Br reaction on an ab initio analytical potential energy surface. Journal of Chemical Physics, 2021, 155, 124301.	1.2	5
15	Vibrational mode-specificity in the dynamics of the Cl + C2H6 â†' HCl + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 114303.	1.2	14
16	Uncovering an oxide ion substitution for the OH^{â˜} + CH₃F reaction. Chemical Science, 2021, 12, 14369-14375.	3.7	17
17	Vibrational mode-specific dynamics of the F(2P3/2) + C2H6 â†' HF + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 154302.	1.2	9
18	High-Level Systematic Ab Initio Comparison of Carbon- and Silicon-Centered S_N2 Reactions. Journal of Physical Chemistry A, 2021, 125, 9645-9657.	1.1	10

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19	Benchmark ab initio and dynamical characterization of the stationary points of reactive atom + alkane and S_N2 potential energy surfaces. Physical Chemistry Chemical Physics, 2020, 22, 4298-4312.	1.3	17
20	Automating the Development of High-Dimensional Reactive Potential Energy Surfaces with the <scp>robosurfer</scp> Program System. Journal of Chemical Theory and Computation, 2020, 16, 51-66.	2.3	60
21	Exact quantum dynamics background of dispersion interactions: case study for CH₄Â·Ar in full (12) dimensions. Physical Chemistry Chemical Physics, 2020, 22, 2792-2802.	1.3	14
22	Rotational Mode Specificity in the F^{â€“} + CH₃I(v = 0, JK) S_N2 and Proton-Transfer Reactions. Journal of Physical Chemistry A, 2020, 124, 8943-8948.	1.1	5
23	Benchmark ab initio characterization of the abstraction and substitution pathways of the OH + CH4/C2H6 reactions. Physical Chemistry Chemical Physics, 2020, 22, 14560-14569.	1.3	16
24	Full-dimensional MRCI-F12 potential energy surface and dynamics of the F(2P3/2) + C2H6 â†' HF + C2H5 reaction. Journal of Chemical Physics, 2020, 153, 064305.	1.2	17
25	Conformers of dehydrogenated glycine isomers. Journal of Computational Chemistry, 2020, 41, 2001-2014.	1.5	13
26	Numerical separation of the front-side attack and double-inversion retention pathways of SN2 reactions. Chemical Physics Letters, 2020, 755, 137780.	1.2	14
27	On the development of a gold-standard potential energy surface for the OH^{â^'} + CH₃I reaction. Physical Chemistry Chemical Physics, 2020, 22, 3775-3778.	1.3	20
28	Theory Finally Agrees with Experiment for the Dynamics of the Cl + C₂H₆ Reaction. Journal of Physical Chemistry Letters, 2020, 11, 4762-4767.	2.1	28
29	Detailed benchmark ab initio mapping of the potential energy surfaces of the X + C2H6 [X = F, Cl, Br, I] reactions. Physical Chemistry Chemical Physics, 2019, 21, 396-408.	1.3	20
30	Uncovering the role of the stationary points in the dynamics of the F^{â^'} + CH₃I reaction. Physical Chemistry Chemical Physics, 2019, 21, 1578-1586.	1.3	13
31	Rethinking the X^{â^'} + CH₃Y [X = OH, SH, CN, NH₂, PH₂; Y = F, Cl, Br, I] S_N2 reactions. Physical Chemistry Chemical Physics, 2019, 21, 7924-7931.	1.3	35
32	Dynamics of proton transfer from ArH+ to CO. International Journal of Mass Spectrometry, 2019, 438, 175-185.	0.7	5
33	High-Level-Optimized Stationary Points for the F^{â€“}(H₂O) + CH₃I System: Proposing a New Water-Induced Double-Inversion Pathway. Journal of Physical Chemistry A, 2019, 123, 454-462.	1.1	10
34	Benchmark ab Initio Characterization of the Complex Potential Energy Surfaces of the X^{â€“} + NH₂Y [X, Y = F, Cl, Br, I] Reactions. Journal of Physical Chemistry A, 2018, 122, 1886-1895.	1.1	16
35	Effects of the Level of Electronic Structure Theory on the Dynamics of the F^{â€“} + CH₃I Reaction. Journal of Physical Chemistry A, 2018, 122, 3353-3364.	1.1	22
36	Mode-Specific Quasiclassical Dynamics of the F^{â€“} + CH₃I S_N2 and Proton-Transfer Reactions. Journal of Physical Chemistry A, 2018, 122, 8143-8151.	1.1	16

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37	Stretching vibration is a spectator in nucleophilic substitution. Science Advances, 2018, 4, eaas9544.	4.7	37
38	Flame Inhibition Chemistry: Rate Coefficients of the Reactions of HBr with CH₃ and OH Radicals at High Temperatures Determined by Quasiclassical Trajectory Calculations. Energy & Fuels, 2018, 32, 10100-10105.	2.5	15
39	Benchmark ab Initio Characterization of the Inversion and Retention Pathways of the OH^{â€“} + CH₃Y [Y = F, Cl, Br, I] S_N2 Reactions. Journal of Physical Chemistry A, 2018, 122, 5773-5780.	1.1	26
40	Deciphering Front-Side Complex Formation in S_N2 Reactions via Dynamics Mapping. Journal of Physical Chemistry Letters, 2017, 8, 2917-2923.	2.1	49
41	Benchmark ab Initio Characterization of the Complex Potential Energy Surface of the F^{â€“} + CH₃CH₂Cl Reaction. Journal of Physical Chemistry A, 2017, 121, 2847-2854.	1.1	25
42	High-level ab initio potential energy surface and dynamics of the F^{â^’}+ CH₃I S_N2 and proton-transfer reactions. Chemical Science, 2017, 8, 3164-3170.	3.7	53
43	Dynamics and Novel Mechanisms of S_N2 Reactions on ab Initio Analytical Potential Energy Surfaces. Journal of Physical Chemistry A, 2017, 121, 9005-9019.	1.1	55
44	Direct mapping of the angle-dependent barrier to reaction for Clâ€‰+â€‰CHD3 using polarized scattering data. Nature Chemistry, 2017, 9, 1175-1180.	6.6	37
45	Does the Cl + CH₄ â†’ H + CH₃Cl Reaction Proceed via Walden Inversion?. Journal of Physical Chemistry A, 2017, 121, 9415-9420.	1.1	10
46	Benchmark ab Initio Characterization of the Complex Potential Energy Surface of the Cl^{â€“} + CH₃I Reaction. Journal of Physical Chemistry A, 2017, 121, 5748-5757.	1.1	23
47	Mode-specific multi-channel dynamics of the Fâ^’ + CHD2Cl reaction on a global ab initio potential energy surface. Journal of Chemical Physics, 2016, 145, 134303.	1.2	15
48	Mode-Specific S_N2 Reaction Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3322-3327.	2.1	63
49	Influence of the leaving group on the dynamics of a gas-phase SN2 reaction. Nature Chemistry, 2016, 8, 151-156.	6.6	116
50	Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Fâ^’ + CH3F SN2 and proton-abstraction reactions. Journal of Chemical Physics, 2015, 142, 244301.	1.2	33
51	Double-Inversion Mechanisms of the X^{â€“} + CH₃Y [X,Y = F, Cl, Br, I] S_N2 Reactions. Journal of Physical Chemistry A, 2015, 119, 3134-3140.	1.1	49
52	Pathways for the OH + Cl2 â†’ HOCl + Cl and HOCl + Cl â†’ HCl + ClO Reactions. Journal of Physical Chemistry A, 2015, 119, 7802-7809.	1.1	5
53	Correlated Dynamics of the O(³P) + CHD₃(v=0) Reaction: A Joint Crossed-Beam and Quasiclassical Trajectory Study. Journal of Physical Chemistry A, 2015, 119, 7190-7196.	1.1	13
54	Revealing a double-inversion mechanism for the Fâ^’+CH3Cl SN2 reaction. Nature Communications, 2015, 6, 5972.	5.8	134

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55	Rotational Mode Specificity in the F^{â€“} + CH₃Y [Y = F and Cl] S_N2 Reactions. Journal of Physical Chemistry A, 2015, 119, 12231-12237.	1.1	9
56	Quasiclassical Trajectory Study of the Rotational Mode Specificity in the O(³P) + CHD₃(v₁ = 0, 1, JK) â†' OH + CD₃ Reactions. Journal of Physical Chemistry A, 2014, 118, 11683-11687.	1.1	17
57	Rotational mode specificity in the Cl + CHD3 â†' HCl + CD3 reaction. Journal of Chemical Physics, 2014, 141, 074310.	1.2	75
58	Communication: Direct comparison between theory and experiment for correlated angular and product-state distributions of the ground-state and stretching-excited O(3P) + CH4 reactions. Journal of Chemical Physics, 2014, 140, 231102.	1.2	11
59	On the Choice of the Ab Initio Level of Theory for Potential Energy Surface Developments. Journal of Physical Chemistry A, 2014, 118, 646-654.	1.1	36
60	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in Small Water and HCl Clusters. Accounts of Chemical Research, 2014, 47, 2700-2709.	7.6	46
61	Reaction Dynamics of Methane with F, O, Cl, and Br on ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 2839-2864.	1.1	96
62	Surprising Quenching of the Spinâ€“Orbit Interaction Significantly Diminishes H₂OÂ·Â·X [X = F, Cl, Br, I] Dissociation Energies. Journal of Physical Chemistry A, 2014, 118, 11956-11961.	1.1	6
63	Quasiclassical Trajectory Studies of the O(³P) + CX₄(v_k = 0, 1) â†' OX(v) + CX₃(n₁n₂n₃n₄) [X = H and D] Reactions on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 6409-6420.	1.1	41
64	Dynamics of the Fâ¯ + CH3Cl â†' Clâ¯ + CH3F SN2 reaction on a chemically accurate potential energy surface. Chemical Science, 2013, 4, 4362.	3.7	70
65	Reduced-Dimensional Quantum Computations for the Rotationalâ€“Vibrational Dynamics of F^{â€“}â€“CH₄ and F^{â€“}â€“CH₂D₂. Journal of Physical Chemistry A, 2013, 117, 6975-6983.	1.1	11
66	Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Br(2P, 2P3/2) + CH4 â†' HBr + CH3 reaction. Journal of Chemical Physics, 2013, 138, 134301.	1.2	36
67	Quantum Dynamics Study of the F + CH₄ â†' HF + CH₃ Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 7124-7130.	1.1	30
68	Translational energy dependence of the Clâ€‰+â€‰CH4(vbâ€‰=â€‰0,â€‰1) reactions: a joint crossed-beam and quasiclassical trajectory study. Molecular Physics, 2012, 110, 1617-1626.	0.8	32
69	Theoretical Study of the Validity of the Polanyi Rules for the Late-Barrier Cl + CHD₃ Reaction. Journal of Physical Chemistry Letters, 2012, 3, 3416-3419.	2.1	106
70	The fourth age of quantum chemistry: molecules in motion. Physical Chemistry Chemical Physics, 2012, 14, 1085-1106.	1.3	196
71	Gaussian Binning of the Vibrational Distributions for the Cl + CH₄(v_{4/2} = 0, 1) â†' H + CH₃Cl(n₁n₂n₃n₄n₅ Reactions. Journal of Physical Chemistry A, 2012, 116, 7467-7473.	1.1	55
72	Temperature-Dependent, Effective Structures of the ¹⁴NH₃ and ¹⁴ND₃ Molecules. Journal of Physical Chemistry A, 2012, 116, 4356-4362.	1.1	8

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73	Mode Selectivity for a â€œCentralâ€•Barrier Reaction: Eight-Dimensional Quantum Studies of the O(³P) + CH₄ â†' OH + CH₃ Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry Letters, 2012, 3, 3776-3780.	2.1	87
74	Dynamics of the O(3P) + CHD3(vCH = 0,1) reactions on an accurate ab initio potential energy surface. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7997-8001.	3.3	78
75	Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Cl(2P, 2P3/2) + CH4 â†' HCl + CH3 and H + CH3Cl reactions. Journal of Chemical Physics, 2012, 136, 044307.	1.2	76
76	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in the Water Dimer. Journal of the American Chemical Society, 2012, 134, 15430-15435.	6.6	89
77	A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements. Journal of Mathematical Chemistry, 2012, 50, 636-651.	0.7	12
78	High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 8094.	1.3	252
79	Communication: Quasiclassical trajectory calculations of correlated product-state distributions for the dissociation of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2011, 135, 151102.	1.2	33
80	An ab initio spinâ€“orbit-corrected potential energy surface and dynamics for the F + CH4 and F + CHD3 reactions. Physical Chemistry Chemical Physics, 2011, 13, 8306.	1.3	47
81	Communication: Probing the entrance channels of the X + CH4 â†' HX + CH3 (X = F, Cl, Br, I) reactions via photodetachment of Xâ¯â€“CH4. Journal of Chemical Physics, 2011, 134, 191102.	1.2	35
82	Dynamics of the Reaction of Methane with Chlorine Atom on an Accurate Potential Energy Surface. Science, 2011, 334, 343-346.	6.0	167
83	Zero-point energy constrained quasiclassical, classical, and exact quantum simulations of isomerizations and radial distribution functions of the water trimer using an ab initio potential energy surface. Chemical Physics Letters, 2010, 500, 217-222.	1.2	31
84	A practical method to avoid zero-point leak in molecular dynamics calculations: Application to the water dimer. Journal of Chemical Physics, 2010, 132, 164103.	1.2	73
85	Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. Journal of Chemical Physics, 2010, 133, 034113.	1.2	61
86	Communication: Experimental and theoretical investigations of the effects of the reactant bending excitations in the F+CHD3 reaction. Journal of Chemical Physics, 2010, 133, 131101.	1.2	46
87	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	2.1	97
88	On the efficiency of treating singularities in triatomic variational vibrational computations. The vibrational states of H+3 up to dissociation. Physical Chemistry Chemical Physics, 2010, 12, 8373.	1.3	33
89	Adiabatic Jacobi corrections on the vibrational energy levels of H2+ isotopologues. Journal of Chemical Physics, 2009, 130, 134314.	1.2	14
90	Toward black-box-type full- and reduced-dimensional variational (ro)vibrational computations. Journal of Chemical Physics, 2009, 130, 134112.	1.2	180

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91	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	1.0	33
92	CH Stretching Excitation Steers the F Atom to the CD Bond in the F + CHD₃ Reaction. Journal of the American Chemical Society, 2009, 131, 17534-17535.	6.6	108
93	Quasiclassical trajectory calculations of correlated product distributions for the F+CHD3(v1=,1) reactions using an ab initio potential energy surface. Journal of Chemical Physics, 2009, 131, 244302.	1.2	190
94	Conformers of gaseous threonine. Molecular Physics, 2009, 107, 761-775.	0.8	43
95	Bridging Theory with Experiment: A Benchmark Study of Thermally Averaged Structural and Effective Spectroscopic Parameters of the Water Molecule. Journal of Physical Chemistry A, 2009, 113, 11665-11678.	1.1	52
96	Accurate ab initio potential energy surface, dynamics, and thermochemistry of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2009, 130, 084301.	1.2	130
97	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	2.3	42
98	Accurate ab Initio Structure, Dissociation Energy, and Vibrational Spectroscopy of the Fâ˜'â˜'CH4 Anion Complex. Journal of Physical Chemistry A, 2008, 112, 7466-7472.	1.1	25
99	Adiabatic Jacobi corrections for H2+-like systems. Journal of Chemical Physics, 2007, 126, 024102.	1.2	6
100	Vibrational energy levels with arbitrary potentials using the Eckart-Watson Hamiltonians and the discrete variable representation. Journal of Chemical Physics, 2007, 127, 084102.	1.2	90
101	Use of a nondirect-product basis for treating singularities in triatomic rotationalâ€“vibrational calculations. Physical Chemistry Chemical Physics, 2007, 9, 3407.	1.3	8
102	Chapter 9 An Active Database Approach to Complete Rotationalâ€“Vibrational Spectra of Small Molecules. Annual Reports in Computational Chemistry, 2007, 3, 155-176.	0.9	54
103	The methylene saga continues: Stretching fundamentals and zero-point energy of CH2. Journal of Molecular Structure, 2006, 780-781, 283-294.	1.8	31
104	Finite basis representations with nondirect product basis functions having structure similar to that of spherical harmonics. Journal of Chemical Physics, 2006, 124, 014110.	1.2	12
105	Treating singularities present in the Sutcliffe-Tennyson vibrational Hamiltonian in orthogonal internal coordinates. Journal of Chemical Physics, 2005, 122, 024101.	1.2	14
106	On equilibrium structures of the water molecule. Journal of Chemical Physics, 2005, 122, 214305.	1.2	157
107	Accurate ab initio determination of spectroscopic and thermochemical properties of mono- and dichlorocarbenes. Physical Chemistry Chemical Physics, 2005, 7, 2881.	1.3	43
108	Variational vibrational calculations using high-order anharmonic force fields. Molecular Physics, 2004, 102, 2411-2423.	0.8	65

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109	On one-dimensional discrete variable representations with general basis functions. Journal of Chemical Physics, 2003, 119, 10512-10518.	1.2	39
110	Conformers of gaseous threonine. , 0, .		1