

Gábor I Csonka

List of Publications by Year in descending order

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105
papers

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76326

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docs citations

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times ranked

14721
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecule-surface interaction from van der Waals-corrected semilocal density functionals: The example of thiophene on transition-metal surfaces. <i>Physical Review Materials</i> , 2020, 4, .	2.4	13
2	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2469-2479.	5.3	26
3	Reference Determinant Dependence of the Random Phase Approximation in 3d Transition Metal Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 100-109.	5.3	15
4	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 796-803.	5.3	25
5	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4753-4764.	5.3	48
6	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. <i>Periodica Polytechnica: Chemical Engineering</i> , 2016, 60, 2-7.	1.1	18
7	Application of a Dual-Hybrid Direct Random Phase Approximation to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4222-4232.	5.3	7
8	Features of the interactions between the methyl-CpG motif and the arginine residues on the surface of MBD proteins. <i>Structural Chemistry</i> , 2016, 27, 1317-1326.	2.0	5
9	Unified picture for the conformation and stabilization of the O-glycosidic linkage in glycopeptide model structures. <i>Structural Chemistry</i> , 2015, 26, 1367-1376.	2.0	5
10	Accurate Complete Basis Set Extrapolation of Direct Random Phase Correlation Energies. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3961-3967.	5.3	9
11	Accurate Diels-Ålder Reaction Energies from Efficient Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2879-2888.	5.3	19
12	Construction and Application of a New Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4615-4626.	5.3	54
13	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anion-π Interaction Energies in Model Structures. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 360-371.	5.3	26
14	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. <i>Physical Review Letters</i> , 2013, 111, 106401.	7.8	168
15	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	5.3	68
16	van der Waals interaction as a summable asymptotic series. <i>Physical Review A</i> , 2012, 86, .	2.5	15
17	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 424207.	1.8	12
18	Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. <i>Physical Review Letters</i> , 2012, 109, 233203.	7.8	66

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19	A meta-GGA Made Free of the Order of Limits Anomaly. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2078-2087.	5.3	49
20	Lattice constants from semilocal density functionals with zero-point phonon correction. <i>Physical Review B</i> , 2012, 85, .	3.2	63
21	Conformational analysis of cellobiose by electronic structure theories. <i>Carbohydrate Research</i> , 2012, 350, 68-76.	2.3	55
22	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. <i>Physical Review B</i> , 2011, 84, .	3.2	180
23	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 988-997.	5.3	26
24	Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. <i>Cellulose</i> , 2011, 18, 897-909.	4.9	18
25	A simple but fully nonlocal correction to the random phase approximation. <i>Journal of Chemical Physics</i> , 2011, 134, 114110.	3.0	33
26	Global Hybrid Functionals: A Look at the Engine under the Hood. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3688-3703.	5.3	87
27	The RPA Atomization Energy Puzzle. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 127-134.	5.3	76
28	Comparison of different force fields for the study of disaccharides. <i>Carbohydrate Research</i> , 2009, 344, 2217-2228.	2.3	87
29	Evaluation of Density Functionals and Basis Sets for Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 679-692.	5.3	183
30	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2950-2958.	5.3	76
31	Regularized Gradient Expansion for Atoms, Molecules, and Solids. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 763-769.	5.3	36
32	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 902-908.	5.3	306
33	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. <i>Physical Review Letters</i> , 2009, 103, 026403.	7.8	507
34	Assessing the performance of recent density functionals for bulk solids. <i>Physical Review B</i> , 2009, 79, .	3.2	740
35	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. <i>Physical Review Letters</i> , 2008, 100, 136406.	7.8	8,139
36	Perdew et al. Reply. <i>Physical Review Letters</i> , 2008, 101, .	7.8	59

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37	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 888-891.	5.3	63
38	Simple charge-transfer model to explain the electrical response of hydrogen chains. <i>Physical Review A</i> , 2008, 78, .	2.5	20
39	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. <i>Physical Review A</i> , 2008, 77, .	2.5	52
40	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H ₂ ⁺ , He ₂ ⁺ , LiH ⁺ , and Ne ₂ ⁺ . <i>Journal of Chemical Physics</i> , 2007, 126, 104102.	3.0	274
41	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. <i>Physical Review A</i> , 2007, 76, .	2.5	37
42	Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. <i>Journal of Chemical Physics</i> , 2007, 126, 244107.	3.0	26
43	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. <i>Philosophical Magazine</i> , 2007, 87, 1071-1084.	1.6	11
44	Exchange and correlation in open systems of fluctuating electron number. <i>Physical Review A</i> , 2007, 76, .	2.5	140
45	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2006, 124, 094108.	3.0	122
46	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. <i>Journal of Chemical Physics</i> , 2006, 125, 194112.	3.0	383
47	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 577-586.	1.8	21
48	Energies of organic molecules and atoms in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 506-511.	2.0	64
49	Proper Gaussian Basis Sets for Density Functional Studies of Water Dimers and Trimers. <i>Journal of Physical Chemistry B</i> , 2005, 109, 21471-21475.	2.6	36
50	Estimation, Computation, and Experimental Correction of Molecular Zero-Point Vibrational Energies. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6779-6789.	2.5	47
51	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11006-11014.	2.5	57
52	Binding Energy Curves from Nonempirical Density Functionals II. van der Waals Bonds in Rare-Gas and Alkaline-Earth Diatomics. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11015-11021.	2.5	82
53	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201.	3.0	769
54	Implicit Zero-Point Vibration Energy and Thermal Corrections in Rapid Estimation of Enthalpies of Formation from Hartree-Fock Total Energy and Partial Charges. <i>Journal of Physical Chemistry A</i> , 2003, 107, 736-744.	2.5	11

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55	Rapid Estimation of Enthalpies of Formation from Hartree-Fock Total Energy and Partial Charges for Compounds Containing Si, S, and Cl Atoms. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8687-8695.	2.5	3
56	Rapid Estimation of Zero-Point Energies of Molecules Using Hartree-Fock Atomic Partial Charges. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1833-1839.	2.5	14
57	Optimal Selection of Partial Charge Calculation Method for Rapid Estimation of Enthalpies of Formation from Hartree-Fock Total Energy. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12139-12150.	2.5	13
58	Ab Initio Conformational Space Study of Model Compounds of O-Glycosides of Serine Diamide. <i>Chemistry - A European Journal</i> , 2002, 8, 4718-4733.	3.3	15
59	Proper basis set for quantum mechanical studies of potential energy surfaces of carbohydrates. <i>Computational and Theoretical Chemistry</i> , 2002, 584, 1-4.	1.5	99
60	Organizing atomic partial charges into a database. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 1-5.	1.5	1
61	Reproducing Gaussian-3 Total Energy Using Fitted Atomic Correlation Parameters for the Rapid Estimation of Correlation Energy from Partial Charges Method and Hartree-Fock Results. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1926-1933.	2.5	16
62	Accurate thermochemistry from corrected Hartree-Fock results: rapid estimation of nearly experimental quality total energy using the small 6-31G(d) basis set. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 319-328.	1.4	19
63	The performance of the rapid estimation of basis set error and correlation energy from partial charges method on new molecules of the G3/99 test set. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 404-411.	1.4	12
64	Fitting atomic correlation parameters for RECEP (rapid estimation of correlation energy from partial) <i>Journal of Computational Chemistry</i> , 2001, 22, 241-254.	3.3	18
65	Prospects in computational molecular medicine: a millennial mega-project on peptide folding. <i>Computational and Theoretical Chemistry</i> , 2000, 500, 5-58.	1.5	29
66	Ab Initio Conformational Study of Two Lewis X Analogues. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7113-7122.	2.5	10
67	Ab Initio Study of Lowest-Energy Conformers of Lewis X (Lex) Trisaccharide. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3381-3390.	2.5	17
68	New development in RECEP (rapid estimation of correlation energy from partial charges) method. <i>Chemical Physics Letters</i> , 1999, 307, 469-478.	2.6	19
69	Comparison of ab initio and density functional methods for vibrational analysis of TeCl ₄ . <i>Journal of Computational Chemistry</i> , 1998, 19, 308-318.	3.3	9
70	Inclusion of exact exchange for self-interaction corrected H ₃ density functional potential energy surface. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 158-165.	1.4	61
71	Theoretical Study of Alternative Ring Forms of α -L-Fucopyranose. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1219-1229.	2.5	26
72	Relative Stability and Structure of Dihydro-1,2,4-triazines: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1998, 63, 5824-5830.	3.2	10

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73	The conformational space of selected aldo-pyrano-hexoses. Computational and Theoretical Chemistry, 1997, 395-396, 29-40.	1.5	26
74	Peptide models XV. The effect of basis set size increase and electron correlation on selected minima of the ab initio 2D-Ramachandran map of For-Gly-NH ₂ and For-L-Ala-NH ₂ . Computational and Theoretical Chemistry, 1997, 391, 15-26.	1.5	66
75	The origin of the problems with the PM3 core repulsion function. Computational and Theoretical Chemistry, 1997, 393, 31-38.	1.5	88
76	Monte Carlo simulation of amorphous systems with the fragment self-consistent field method. Computational and Theoretical Chemistry, 1997, 398-399, 129-133.	1.5	3
77	Flexible ab initio geometry of methylamine and its internal rotation. Journal of Molecular Structure, 1997, 410-411, 387-390.	3.6	1
78	Ab initio and density functional study of the conformational space of 1C ₄ ?-L-fucose. Journal of Computational Chemistry, 1997, 18, 330-342.	3.3	38
79	Simple tests for density functional methods. Journal of Computational Chemistry, 1997, 18, 1534-1545.	3.3	25
80	Vibrational analysis of TeCl ₄ . II. A Hartree-Fock, MP2, and density functional study. International Journal of Quantum Chemistry, 1997, 65, 817-826.	2.0	5
81	Prediction of geometrical parameters for silatranes: an ab initio molecular orbital and density functional theory study. Computational and Theoretical Chemistry, 1996, 362, 199-208.	1.5	26
82	Vibrational properties of C ₂₀ isomers, a semi-empirical study. Journal of Molecular Structure, 1996, 376, 513-523.	3.6	10
83	The structure of 1-chlorosilatrane: An ab initio molecular orbital and a density functional theory study. Journal of Computational Chemistry, 1996, 17, 767-780.	3.3	21
84	Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. Journal of Computational Chemistry, 1996, 17, 1804-1819.	3.3	24
85	Relative stability of 1C ₄ and 4C ₁ chair forms of β -D-glucose: a density functional study. Chemical Physics Letters, 1996, 257, 49-60.	2.6	81
86	Density functional and post Hartree-Fock equilibrium geometries, potential energy surface and vibrational frequencies for methylamine. Chemical Physics Letters, 1995, 233, 611-618.	2.6	18
87	Density functional conformational analysis of 1,2-ethanediol. Chemical Physics Letters, 1995, 243, 419-428.	2.6	46
88	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. Chemical Physics Letters, 1995, 245, 129-135.	2.6	28
89	The photoelectron spectrum and conformation of phenylphosphine and phenylarsine. Structural Chemistry, 1995, 6, 1-7.	2.0	22
90	The failure of the MO-based theoretical explanations for bending of disiloxane. Computational and Theoretical Chemistry, 1995, 332, 187-188.	1.5	4

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91	Ab initio prediction of gas phase molecular structure of 1-chlorosilatrane. AIP Conference Proceedings, 1995, , .	0.4	0
92	Structure of disiloxane: Semiempirical and post-Hartree-Fock study. AIP Conference Proceedings, 1995, , .	0.4	0
93	Density functional study of the equilibrium geometry and Si-O-Si potential energy curve of disiloxane. Chemical Physics Letters, 1994, 229, 191-197.	2.6	32
94	Ab initio molecular orbital study of 1-fluorosilatrane. Journal of Computational Chemistry, 1994, 15, 385-394.	3.3	28
95	Structure of disiloxane: A semiempirical and Post-Hartree-Fock study. Journal of Computational Chemistry, 1994, 15, 925-936.	3.3	21
96	Analysis of the core-repulsion functions used in AM1 and PM3 semiempirical calculations: Conformational analysis of ring systems. Journal of Computational Chemistry, 1993, 14, 895-898.	3.3	52
97	Wavenumbers and intensities of the fundamental vibrational modes of HNSi and DNSi from quantum-chemical computations. Journal of Molecular Structure, 1993, 297, 243-253.	3.6	1
98	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. Journal of Organometallic Chemistry, 1993, 454, 15-23.	1.8	20
99	MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. Journal of Organometallic Chemistry, 1993, 446, 99-106.	1.8	22
100	Investigation of heterocyclic compounds containing a $\text{P}\hat{\text{i}}\text{---}\text{C}$ or $\text{As}\hat{\text{i}}\text{---}\text{C}$ bond by ultraviolet photoelectron spectroscopy. Journal of Organometallic Chemistry, 1989, 373, 49-55.	1.8	52
101	Recent advances in fuzzy peak tracking in high-performance liquid chromatography. Journal of Chromatography A, 1989, 485, 557-567.	3.7	13
102	Investigation of 3-substituted benzazaphospholes and benzazarsoles by UV-photoelectron spectroscopy. Journal of Organometallic Chemistry, 1989, 373, 57-61.	1.8	23
103	The molecular structure of 1-phenylsilatranone. Journal of Organometallic Chemistry, 1987, 329, 305-311.	1.8	9
104	Theory of Correlation Tables. 1. Journal of Chemical Information and Computer Sciences, 1980, 20, 234-238.	2.8	1
105	Theory of Correlation Tables. 2. Journal of Chemical Information and Computer Sciences, 1980, 20, 239-241.	2.8	1