GÃ¡bor I Csonka

List of Publications by Year
in descending order

105	15,155	76196	26548
papers	citations	40 h-index	107 g-index

111	111	111	14721
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	2.9	8,139
2	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. Journal of Chemical Physics, 2005, 123, 062201.	1.2	769
3	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	1.1	740
4	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403.	2.9	507
5	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. Journal of Chemical Physics, 2006, 125, 194112.	1.2	383
6	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	2.3	306
7	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H2+, He2+, LiH+, and Ne2+. Journal of Chemical Physics, 2007, 126, 104102.	1.2	274
8	Evaluation of Density Functionals and Basis Sets for Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 679-692.	2.3	183
9	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180
10	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	2.9	168
11	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	1.0	140
12	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108.	1.2	122
13	Proper basis set for quantum mechanical studies of potential energy surfaces of carbohydrates. Computational and Theoretical Chemistry, 2002, 584, 1-4.	1.5	99
14	The origin of the problems with the PM3 core repulsion function. Computational and Theoretical Chemistry, 1997, 393, 31-38.	1.5	88
15	Comparison of different force fields for the study of disaccharides. Carbohydrate Research, 2009, 344, 2217-2228.	1.1	87
16	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
17	Binding Energy Curves from Nonempirical Density Functionals II. van der Waals Bonds in Rare-Gas and Alkaline-Earth Diatomics. Journal of Physical Chemistry A, 2005, 109, 11015-11021.	1.1	82
18	Relative stability of 1C4 and 4C1 chair forms of Î²-d-glucose: a density functional study. Chemical Physics Letters, 1996, 257, 49-60.	1.2	81

#	Article	IF	Citations
19	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2950-2958.	2.3	76
20	The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134.	2.3	76
21	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 355-363.	2.3	68
22	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-NH2 and For-l-Ala-NH2. Computational and Theoretical Chemistry, 1997, 391, 15-26.	1.5	66
23	Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. Physical Review Letters, 2012, 109, 233203.	2.9	66
24	Energies of organic molecules and atoms in density functional theory. International Journal of Quantum Chemistry, 2005, 101, 506-511.	1.0	64
25	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 888-891.	2.3	63
26	Lattice constants from semilocal density functionals with zero-point phonon correction. Physical Review B, 2012, 85, .	1.1	63
27	Inclusion of exact exchange for self-interaction corrected H 3 density functional potential energy surface. Theoretical Chemistry Accounts, 1998, 99, 158-165.	0.5	61
28	PerdewetÂal.Reply:. Physical Review Letters, 2008, 101, .	2.9	59
29	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. Journal of Physical Chemistry A, 2005, 109, 11006-11014.	1.1	57
30	Conformational analysis of cellobiose by electronic structure theories. Carbohydrate Research, 2012, 350, 68-76.	1.1	55
31	Construction and Application of a New Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2015, 11, 4615-4626.	2.3	54
32	Investigation of heterocyclic compounds containing a Pî—»C or Asî—»C bond by ultraviolet photoelectron spectroscopy. Journal of Organometallic Chemistry, 1989, 373, 49-55.	0.8	52
33	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.	1.5	52
34	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, .	1.0	52
35	A meta-GGA Made Free of the Order of Limits Anomaly. Journal of Chemical Theory and Computation, 2012, 8, 2078-2087.	2.3	49
36	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. Journal of Chemical Theory and Computation, 2017, 13, 4753-4764.	2.3	48

#	ARTICLE	IF	CITATIONS
37	Estimation, Computation, and Experimental Correction of Molecular Zero-Point Vibrational Energies. Journal of Physical Chemistry A, 2005, 109, 6779-6789.	1.1	47
38	Density functional conformational analysis of 1,2-ethanediol. Chemical Physics Letters, 1995, 243, 419-428.	1.2	46
39	Ab initio and density functional study of the conformational space of1C4 ?-L-fucose. Journal of Computational Chemistry, 1997, 18, 330-342.	1.5	38
40	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	1.0	37
41	Proper Gaussian Basis Sets for Density Functional Studies of Water Dimers and Trimers. Journal of Physical Chemistry B, 2005, 109, 21471-21475.	1.2	36
42	Regularized Gradient Expansion for Atoms, Molecules, and Solids. Journal of Chemical Theory and Computation, 2009, 5, 763-769.	2.3	36
43	A simple but fully nonlocal correction to the random phase approximation. Journal of Chemical Physics, 2011, 134, 114110.	1.2	33
44	Density functional study of the equilibrium geometry and Si-O-Si potential energy curve of disiloxane. Chemical Physics Letters, 1994, 229, 191-197.	1.2	32
45	Prospects in computational molecular medicine: a millennial mega-project on peptide folding. Computational and Theoretical Chemistry, 2000, 500, 5-58.	1.5	29
46	Ab initio molecular orbital study of 1-fluorosilatrane. Journal of Computational Chemistry, 1994, 15, 385-394.	1.5	28
47	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. Chemical Physics Letters, 1995, 245, 129-135.	1.2	28
48	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
49	The conformational space of selected aldo-pyrano-hexoses. Computational and Theoretical Chemistry, 1997, 395-396, 29-40.	1.5	26
50	Theoretical Study of Alternative Ring Forms of Î±-l-Fucopyranose. Journal of Physical Chemistry A, 1998, 102, 1219-1229.	1.1	26
51	Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. Journal of Chemical Physics, 2007, 126, 244107.	1.2	26
52	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. Journal of Chemical Theory and Computation, 2011, 7, 988-997.	2.3	26
53	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anionâ˜Ï€ Interaction Energies in Model Structures. Journal of Chemical Theory and Computation, 2015, 11, 360-371.	2.3	26
54	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. Journal of Chemical Theory and Computation, 2018, 14, 2469-2479.	2.3	26

#	ARTICLE	IF	CITATIONS
55	Simple tests for density functional methods. Journal of Computational Chemistry, 1997, 18, 1534-1545.	1.5	25
56	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2017, 13, 796-803.	2.3	25
57	Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. Journal of Computational Chemistry, 1996, 17, 1804-1819.	1.5	24
58	Investigation of 3-substituted benzazaphospholes and benzazarsoles by UV-photoelectron spectroscopy. Journal of Organometallic Chemistry, 1989, 373, 57-61.	0.8	23
59	MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. Journal of Organometallic Chemistry, 1993, 446, 99-106.	0.8	22
60	The photoelectron spectrum and conformation of phenylphosphine and phenylarsine. Structural Chemistry, 1995, 6, 1-7.	1.0	22
61	Structure of disiloxane: A semiempirical and Post-Hartree-Fock study. Journal of Computational Chemistry, 1994, 15, 925-936.	1.5	21
62	The structure of 1-chlorosilatrane: Anab initio molecular orbital and a density functional theory study. Journal of Computational Chemistry, 1996, 17, 767-780.	1.5	21
63	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. Tetrahedron: Asymmetry, 2005, 16, 577-586.	1.8	21
64	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. Journal of Organometallic Chemistry, 1993, 454, 15-23.	0.8	20
65	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	1.0	20
66	New development in RECEP (rapid estimation of correlation energy from partial charges) method. Chemical Physics Letters, 1999, 307, 469-478.	1.2	19
67	Accurate thermochemistry from corrected Hartree-Fock results: rapid estimation of nearly experimental quality total energy using the small 6-31G(d) basis set. Theoretical Chemistry Accounts, 2001, 106, 319-328.	0.5	19
68	Accurate Dielsâ€“Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888.	2.3	19
69	Density functional and post Hartree-Fock equilibrium geometries, potential energy surface and vibrational frequencies for methylamine. Chemical Physics Letters, 1995, 233, 611-618.	1.2	18
70	Fitting atomic correlation parameters for RECEP (rapid estimation of correlation energy from partial) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Computational Chemistry, 2001, 22, 241-254.	1.5	18
71	Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. Cellulose, 2011, 18, 897-909.	2.4	18
72	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. Periodica Polytechnica: Chemical Engineering, 2016, 60, 2-7.	0.5	18

#	ARTICLE	IF	CITATIONS
73	Ab Initio Study of Lowest-Energy Conformers of Lewis X (Lex) Trisaccharide. Journal of Physical Chemistry A, 2000, 104, 3381-3390.	1.1	17
74	Reproducing Gaussian-3 Total Energy Using Fitted Atomic Correlation Parameters for the Rapid Estimation of Correlation Energy from Partial Charges Method and Hartreeâ^'Fock Results. Journal of Physical Chemistry A, 2001, 105, 1926-1933.	1.1	16
75	Ab Initio Conformational Space Study of Model Compounds of O-Glycosides of Serine Diamide. Chemistry - A European Journal, 2002, 8, 4718-4733.	1.7	15
76	van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, .	1.0	15
77	Reference Determinant Dependence of the Random Phase Approximation in 3d Transition Metal Chemistry. Journal of Chemical Theory and Computation, 2017, 13, 100-109.	2.3	15
78	Rapid Estimation of Zero-Point Energies of Molecules Using Hartreeâ^'Fock Atomic Partial Charges. Journal of Physical Chemistry A, 2003, 107, 1833-1839.	1.1	14
79	Recent advances in fuzzy peak tracking in high-performance liquid chromatography. Journal of Chromatography A, 1989, 485, 557-567.	1.8	13
80	Optimal Selection of Partial Charge Calculation Method for Rapid Estimation of Enthalpies of Formation from Hartreeâ^'Fock Total Energy. Journal of Physical Chemistry A, 2002, 106, 12139-12150.	1.1	13
81	Molecule-surface interaction from van der Waals-corrected semilocal density functionals: The example of thiophene on transition-metal surfaces. Physical Review Materials, 2020, 4, .	0.9	13
82	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. Theoretical Chemistry Accounts, 2001, 106, 404-411.	0.5	12
83	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. Journal of Physics Condensed Matter, 2012, 24, 424207.	0.7	12
84	Implicit Zero-Point Vibration Energy and Thermal Corrections in Rapid Estimation of Enthalpies of Formation from Hartreeâ^'Fock Total Energy and Partial Charges. Journal of Physical Chemistry A, 2003, 107, 736-744.	1.1	11
85	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. Philosophical Magazine, 2007, 87, 1071-1084.	0.7	11
86	Vibrational properties of C20 isomers, a semi-empirical study. Journal of Molecular Structure, 1996, 376, 513-523.	1.8	10
87	Relative Stability and Structure of Dihydro-1,2,4-triazines:â€‰ A Theoretical Study. Journal of Organic Chemistry, 1998, 63, 5824-5830.	1.7	10
88	Ab Initio Conformational Study of Two Lewis X Analogues. Journal of Physical Chemistry A, 2000, 104, 7113-7122.	1.1	10
89	The molecular structure of 1-phenylsilatranone. Journal of Organometallic Chemistry, 1987, 329, 305-311.	0.8	9
90	Comparison ofab initio and density functional methods for vibrational analysis of TeCl4. Journal of Computational Chemistry, 1998, 19, 308-318.	1.5	9

#	ARTICLE	IF	CITATIONS
91	Accurate Complete Basis Set Extrapolation of Direct Random Phase Correlation Energies. Journal of Chemical Theory and Computation, 2015, 11, 3961-3967.	2.3	9
92	Application of a Dual-Hybrid Direct Random Phase Approximation to Water Clusters. Journal of Chemical Theory and Computation, 2016, 12, 4222-4232.	2.3	7
93	Vibrational analysis of TeCl4. II. A Hartree-Fock, MP2, and density functional study. International Journal of Quantum Chemistry, 1997, 65, 817-826.	1.0	5
94	Unified picture for the conformation and stabilization of the O-glycosidic linkage in glycopeptide model structures. Structural Chemistry, 2015, 26, 1367-1376.	1.0	5
95	Features of the interactions between the methyl-CpG motif and the arginine residues on the surface of MBD proteins. Structural Chemistry, 2016, 27, 1317-1326.	1.0	5
96	The failure of the MO-based theoretical explanations for bending of disiloxane. Computational and Theoretical Chemistry, 1995, 332, 187-188.	1.5	4
97	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
98	Rapid Estimation of Enthalpies of Formation from Hartreeâ^'Fock Total Energy and Partial Charges for Compounds Containing Si, S, and Cl Atoms. Journal of Physical Chemistry A, 2003, 107, 8687-8695.	1.1	3
99	Theory of Correlation Tables. 1. Journal of Chemical Information and Computer Sciences, 1980, 20, 234-238.	2.8	1
100	Theory of Correlation Tables. 2. Journal of Chemical Information and Computer Sciences, 1980, 20, 239-241.	2.8	1
101	Wavenumbers and intensities of the fundamental vibrational modes of HNSi and DNSi from quantum-chemical computations. Journal of Molecular Structure, 1993, 297, 243-253.	1.8	1
102	Flexible ab initio geometry of methylamine and its internal rotation. Journal of Molecular Structure, 1997, 410-411, 387-390.	1.8	1
103	Organizing atomic partial charges into a database. Computational and Theoretical Chemistry, 2002, 589-590, 1-5.	1.5	1
104	Ab initio prediction of gas phase molecular structure of 1-chlorsilatrane. AIP Conference Proceedings, 1995, , .	0.3	0
105	Structure of disiloxane: Semiempirical and post-Hartree-Fock study. AIP Conference Proceedings, 1995, , .	0.3	0