

# Gbor I Csonka

## List of Publications by Citations

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102  
papers

12,008  
citations

39  
h-index

109  
g-index

111  
ext. papers

13,548  
ext. citations

3.8  
avg, IF

6.01  
L-index

#	Paper	IF	Citations
102	Restoring the density-gradient expansion for exchange in solids and surfaces. <i>Physical Review Letters</i> , <b>2008</b> , 100, 136406	7.4	5934
101	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 62201	3.9	658
100	Assessing the performance of recent density functionals for bulk solids. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	530
99	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. <i>Physical Review Letters</i> , <b>2009</b> , 103, 026403	7.4	426
98	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 194112	3.9	349
97	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 902-8	6.4	273
96	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H <sub>2</sub> <sup>+</sup> , He <sub>2</sub> <sup>+</sup> , LiH <sup>+</sup> , and Ne <sub>2</sub> <sup>+</sup> . <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 104102	3.9	248
95	Evaluation of Density Functionals and Basis Sets for Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 679-92	6.4	157
94	Density functionals that recognize covalent, metallic, and weak bonds. <i>Physical Review Letters</i> , <b>2013</b> , 111, 106401	7.4	143
93	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	138
92	Exchange and correlation in open systems of fluctuating electron number. <i>Physical Review A</i> , <b>2007</b> , 76,	2.6	131
91	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 94108	3.9	108
90	Proper basis set for quantum mechanical studies of potential energy surfaces of carbohydrates. <i>Computational and Theoretical Chemistry</i> , <b>2002</b> , 584, 1-4		87
89	The origin of the problems with the PM3 core repulsion function. <i>Computational and Theoretical Chemistry</i> , <b>1997</b> , 393, 31-38		80
88	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> , <b>2005</b> , 109, 11015-21	2.8	79
87	Comparison of different force fields for the study of disaccharides. <i>Carbohydrate Research</i> , <b>2009</b> , 344, 2217-28	2.9	78
86	Relative stability of 1C <sub>4</sub> and 4C <sub>1</sub> chair forms of D-glucose: a density functional study. <i>Chemical Physics Letters</i> , <b>1996</b> , 257, 49-60	2.5	78

85	Global Hybrid Functionals: A Look at the Engine under the Hood. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 3688-3703	6.4	77
84	The RPA Atomization Energy Puzzle. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 127-34	6.4	70
83	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2950-8	6.4	70
82	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 355-63	6.4	62
81	Van der waals coefficients for nanostructures: fullerenes defy conventional wisdom. <i>Physical Review Letters</i> , <b>2012</b> , 109, 233203	7.4	62
80	Energies of organic molecules and atoms in density functional theory. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 101, 506-511	2.1	62
79	Inclusion of exact exchange for self-interaction corrected H3 density functional potential energy surface. <i>Theoretical Chemistry Accounts</i> , <b>1998</b> , 99, 158-165	1.9	59
78	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 <sub>2</sub> and For-l-Ala-NH <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , <b>1997</b> , 391, 15-26		58
77	Perdew et al. Reply:. <i>Physical Review Letters</i> , <b>2008</b> , 101,	7.4	55
76	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 888-91	6.4	55
75	Binding energy curves from nonempirical density functionals. I. Covalent bonds in closed-shell and radical molecules. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 11006-14	2.8	53
74	Lattice constants from semilocal density functionals with zero-point phonon correction. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	52
73	Investigation of heterocyclic compounds containing a P?C or As?C bond by ultraviolet photoelectron spectroscopy. <i>Journal of Organometallic Chemistry</i> , <b>1989</b> , 373, 49-55	2.3	49
72	Construction and application of a new dual-hybrid random phase approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 4615-26	6.4	48
71	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. <i>Physical Review A</i> , <b>2008</b> , 77,	2.6	48
70	Conformational analysis of cellobiose by electronic structure theories. <i>Carbohydrate Research</i> , <b>2012</b> , 350, 68-76	2.9	46
69	Density functional conformational analysis of 1,2-ethanediol. <i>Chemical Physics Letters</i> , <b>1995</b> , 243, 419-428	5	45
68	Analysis of the core-repulsion functions used in AM1 and PM3 semiempirical calculations: Conformational analysis of ring systems. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 895-898	3.5	45

67	A meta-GGA Made Free of the Order of Limits Anomaly. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2078-87	6.4	44
66	Estimation, computation, and experimental correction of molecular zero-point vibrational energies. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 6779-89	2.8	42
65	Ab initio and density functional study of the conformational space of 1C4 $\beta$ -D-fucose. <i>Journal of Computational Chemistry</i> , <b>1997</b> , 18, 330-342	3.5	37
64	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. <i>Physical Review A</i> , <b>2007</b> , 76,	2.6	37
63	Regularized Gradient Expansion for Atoms, Molecules, and Solids. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 763-9	6.4	34
62	Proper gaussian basis sets for density functional studies of water dimers and trimers. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 21471-5	3.4	34
61	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4753-4764	6.4	33
60	A simple but fully nonlocal correction to the random phase approximation. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 114110	3.9	31
59	Density functional study of the equilibrium geometry and Si-O-Si potential energy curve of disiloxane. <i>Chemical Physics Letters</i> , <b>1994</b> , 229, 191-197	2.5	27
58	The conformational space of selected aldo-pyrano-hexoses. <i>Computational and Theoretical Chemistry</i> , <b>1997</b> , 395-396, 29-40		26
57	Prospects in computational molecular medicine: a millennial mega-project on peptide folding. <i>Computational and Theoretical Chemistry</i> , <b>2000</b> , 500, 5-58		26
56	Theoretical Study of Alternative Ring Forms of $\beta$ -D-Fucopyranose. <i>Journal of Physical Chemistry A</i> , <b>1998</b> , 102, 1219-1229	2.8	26
55	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. <i>Chemical Physics Letters</i> , <b>1995</b> , 245, 129-135	2.5	26
54	Diminished gradient dependence of density functionals: constraint satisfaction and self-interaction correction. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 244107	3.9	25
53	Ab initio molecular orbital study of 1-fluorosilatrane. <i>Journal of Computational Chemistry</i> , <b>1994</b> , 15, 385-394		25
52	Prediction of geometrical parameters for silatranes: an ab initio molecular orbital and density functional theory study. <i>Computational and Theoretical Chemistry</i> , <b>1996</b> , 362, 199-208		24
51	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 796-803	6.4	23
50	Accurate, precise, and efficient theoretical methods to calculate anion- $\pi$ interaction energies in model structures. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 360-71	6.4	23

49	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 2469-2479	6.4	23
48	Simple tests for density functional methods. <i>Journal of Computational Chemistry</i> , <b>1997</b> , 18, 1534-1545	3.5	22
47	1,3-Dipolare cycloadditionen von 6,7-dialkoxy-3,4-dihydroisochinolinium-Salzen. <i>Tetrahedron</i> , <b>1984</b> , 40, 369-375	2.4	22
46	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 988-97	6.4	21
45	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. <i>Tetrahedron: Asymmetry</i> , <b>2005</b> , 16, 577-586		21
44	The structure of 1-chlorosilatrane: An ab initio molecular orbital and a density functional theory study. <i>Journal of Computational Chemistry</i> , <b>1996</b> , 17, 767-780	3.5	21
43	Structure of disiloxane: A semiempirical and Post-Hartree-Fock study. <i>Journal of Computational Chemistry</i> , <b>1994</b> , 15, 925-936	3.5	21
42	MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. <i>Journal of Organometallic Chemistry</i> , <b>1993</b> , 446, 99-106	2.3	21
41	Investigation of 3-substituted benzazaphospholes and benzazarsoles by UV-photoelectron spectroscopy. <i>Journal of Organometallic Chemistry</i> , <b>1989</b> , 373, 57-61	2.3	21
40	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. <i>Journal of Organometallic Chemistry</i> , <b>1993</b> , 454, 15-23	2.3	20
39	Simple charge-transfer model to explain the electrical response of hydrogen chains. <i>Physical Review A</i> , <b>2008</b> , 78,	2.6	19
38	The photoelectron spectrum and conformation of phenylphosphine and phenylarsine. <i>Structural Chemistry</i> , <b>1995</b> , 6, 1-7	1.8	19
37	Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. <i>Journal of Computational Chemistry</i> , <b>1996</b> , 17, 1804-1819	3.5	19
36	Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. <i>Cellulose</i> , <b>2011</b> , 18, 897-909	5.5	18
35	Fitting atomic correlation parameters for RECEP (rapid estimation of correlation energy from partial charges) method to estimate molecular correlation energies within chemical accuracy. <i>Journal of Computational Chemistry</i> , <b>2001</b> , 22, 241-254	3.5	18
34	New development in RECEP (rapid estimation of correlation energy from partial charges) method. <i>Chemical Physics Letters</i> , <b>1999</b> , 307, 469-478	2.5	18
33	Accurate Diels-Alder reaction energies from efficient density functional calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2879-88	6.4	17
32	Ab Initio Study of Lowest-Energy Conformers of Lewis X (Lex) Trisaccharide. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 3381-3390	2.8	17

31	Density functional and post Hartree-Fock equilibrium geometries, potential energy surface and vibrational frequencies for methylamine. <i>Chemical Physics Letters</i> , <b>1995</b> , 233, 611-618	2.5	17
30	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. <i>Periodica Polytechnica: Chemical Engineering</i> , <b>2016</b> , 60, 2-7	1.3	17
29	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> , <b>2001</b> , 106, 319-328	1.9	16
28	van der Waals interaction as a summable asymptotic series. <i>Physical Review A</i> , <b>2012</b> , 86,	2.6	15
27	Ab initio conformational space study of model compounds of O-glycosides of serine diamide. <i>Chemistry - A European Journal</i> , <b>2002</b> , 8, 4718-33	4.8	15
26	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> , <b>2001</b> , 105, 1926-1933	2.8	15
25	Reference Determinant Dependence of the Random Phase Approximation in 3d Transition Metal Chemistry. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 100-109	6.4	13
24	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 424207	1.8	12
23	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> , <b>2001</b> , 106, 404-411	1.9	12
22	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> , <b>2002</b> , 106, 12139-12150	2.8	12
21	Molecule-surface interaction from van der Waals-corrected semilocal density functionals: The example of thiophene on transition-metal surfaces. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	12
20	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. <i>Philosophical Magazine</i> , <b>2007</b> , 87, 1071-1084	1.6	11
19	Rapid Estimation of Zero-Point Energies of Molecules Using Hartree-Fock Atomic Partial Charges. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 1833-1839	2.8	11
18	Ab Initio Conformational Study of Two Lewis X Analogues. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 7113-7122	2.8	10
17	Vibrational properties of C20 isomers, a semi-empirical study. <i>Journal of Molecular Structure</i> , <b>1996</b> , 376, 513-523	3.4	10
16	Accurate Complete Basis Set Extrapolation of Direct Random Phase Correlation Energies. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 3961-7	6.4	9
15	Comparison of ab initio and density functional methods for vibrational analysis of TeCl4. <i>Journal of Computational Chemistry</i> , <b>1998</b> , 19, 308-318	3.5	9
14	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> , <b>2003</b> , 107, 736-744	2.8	9

13	The molecular structure of 1-phenylsilatranone. <i>Journal of Organometallic Chemistry</i> , <b>1987</b> , 329, 305-311	2.3	9
12	Recent advances in fuzzy peak tracking in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , <b>1989</b> , 485, 557-567	4.5	7
11	Application of a Dual-Hybrid Direct Random Phase Approximation to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4222-32	6.4	7
10	Features of the interactions between the methyl-CpG motif and the arginine residues on the surface of MBD proteins. <i>Structural Chemistry</i> , <b>2016</b> , 27, 1317-1326	1.8	5
9	Unified picture for the conformation and stabilization of the O-glycosidic linkage in glycopeptide model structures. <i>Structural Chemistry</i> , <b>2015</b> , 26, 1367-1376	1.8	5
8	Vibrational analysis of TeCl <sub>4</sub> . II. A Hartree-Fock, MP2, and density functional study. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 65, 817-826	2.1	5
7	Relative Stability and Structure of Dihydro-1,2,4-triazines: A Theoretical Study. <i>Journal of Organic Chemistry</i> , <b>1998</b> , 63, 5824-5830	4.2	5
6	The failure of the MO-based theoretical explanations for bending of disiloxane. <i>Computational and Theoretical Chemistry</i> , <b>1995</b> , 332, 187-188		4
5	Monte Carlo simulation of amorphous systems with the fragment self-consistent field method. <i>Computational and Theoretical Chemistry</i> , <b>1997</b> , 398-399, 129-133		3
4	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> , <b>2003</b> , 107, 8687-8695	2.8	3
3	Flexible ab initio geometry of methylamine and its internal rotation. <i>Journal of Molecular Structure</i> , <b>1997</b> , 410-411, 387-390	3.4	1
2	Organizing atomic partial charges into a database. <i>Computational and Theoretical Chemistry</i> , <b>2002</b> , 589-590, 1-5		1
1	Wavenumbers and intensities of the fundamental vibrational modes of HNSi and DNSi from quantum-chemical computations. <i>Journal of Molecular Structure</i> , <b>1993</b> , 297, 243-253	3.4	1