# 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 | 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 |
| 2 | Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. Journal of Chemical Theory and Computation, 2018, 14, 2469-2479. | 2.3 | 26 |
| 3 | 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 |
| 4 | Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2017, 13, 796-803. | 2.3 | 25 |
| 5 | 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 |
| 6 | Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. Periodica Polytechnica: Chemical Engineering, 2016, 60, 2-7. | 0.5 | 18 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | Accurate Complete Basis Set Extrapolation of Direct Random Phase Correlation Energies. Journal of Chemical Theory and Computation, 2015, 11, 3961-3967. | 2.3 | 9 |
| 11 | Accurate Dielsâ€“Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888. | 2.3 | 19 |
| 12 | Construction and Application of a New Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2015, 11, 4615-4626. | 2.3 | 54 |
| 13 | 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 |
| 14 | Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401. | 2.9 | 168 |
| 15 | 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 |
| 16 | van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, . | 1.0 | 15 |
| 17 | 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 |
| 18 | Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. Physical Review Letters, 2012, 109, 233203. | 2.9 | 66 |

| # | Article | IF | Citations |
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| 19 | A meta-GGA Made Free of the Order of Limits Anomaly. Journal of Chemical Theory and Computation, 2012, 8, 2078-2087. | 2.3 | 49 |
| 20 | Lattice constants from semilocal density functionals with zero-point phonon correction. Physical Review B, 2012, 85, . | 1.1 | 63 |
| 21 | Conformational analysis of cellobiose by electronic structure theories. Carbohydrate Research, 2012, 350, 68-76. | 1.1 | 55 |
| 22 | Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, . | 1.1 | 180 |
| 23 | Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. Journal of Chemical Theory and Computation, 2011, 7, 988-997. | 2.3 | 26 |
| 24 | Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. Cellulose, 2011, 18, 897-909. | 2.4 | 18 |
| 25 | A simple but fully nonlocal correction to the random phase approximation. Journal of Chemical Physics, 2011, 134, 114110. | 1.2 | 33 |
| 26 | Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703. | 2.3 | 87 |
| 27 | The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134. | 2.3 | 76 |
| 28 | Comparison of different force fields for the study of disaccharides. Carbohydrate Research, 2009, 344, 2217-2228. | 1.1 | 87 |
| 29 | Evaluation of Density Functionals and Basis Sets for Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 679-692. | 2.3 | 183 |
| 30 | 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 |
| 31 | Regularized Gradient Expansion for Atoms, Molecules, and Solids. Journal of Chemical Theory and Computation, 2009, 5, 763-769. | 2.3 | 36 |
| 32 | 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 |
| 33 | Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403. | 2.9 | 507 |
| 34 | Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, . | 1.1 | 740 |
| 35 | Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406. | 2.9 | 8,139 |
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| 37 | 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 |
| 38 | Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, . | 1.0 | 20 |
| 39 | Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, . | 1.0 | 52 |
| 40 | 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 |
| 41 | One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, . | 1.0 | 37 |
| 42 | Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. Journal of Chemical Physics, 2007, 126, 244107. | 1.2 | 26 |
| 43 | Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. Philosophical Magazine, 2007, 87, 1071-1084. | 0.7 | 11 |
| 44 | Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, . | 1.0 | 140 |
| 45 | Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108. | 1.2 | 122 |
| 46 | 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 |
| 47 | Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. Tetrahedron: Asymmetry, 2005, 16, 577-586. | 1.8 | 21 |
| 48 | Energies of organic molecules and atoms in density functional theory. International Journal of Quantum Chemistry, 2005, 101, 506-511. | 1.0 | 64 |
| 49 | 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 |
| 50 | Estimation, Computation, and Experimental Correction of Molecular Zero-Point Vibrational Energies. Journal of Physical Chemistry A, 2005, 109, 6779-6789. | 1.1 | 47 |
| 51 | 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 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | 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 |
| 56 | 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 |
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| 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. Theoretical Chemistry Accounts, 2001, 106, 404-411. | 0.5 | 12 |
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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 |
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| 84 | Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. Journal of Computational Chemistry, 1996, 17, 1804-1819. | 1.5 | 24 |
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| 86 | 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 |
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