Jerzy Cioslowski

List of Publications by Year
in descending order

118	3,157	172386	182361
papers	citations	29 h-index	51 g-index

119	119	119	1844
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Endohedral complexes: Atoms and ions inside the C60 cage. Journal of Chemical Physics, 1991, 94, 3730-3734.	1.2	276
2	Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.	1.1	118
3	The ground state of harmonium. Journal of Chemical Physics, 2000, 113, 8434-8443.	1.2	115
4	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
5	A set of standard enthalpies of formation for benchmarking, calibration, and parametrization of electronic structure methods. Journal of Chemical Physics, 2000, 113, 9377-9389.	1.2	105
6	Standard Enthalpies of Formation of Fullerenes and Their Dependence on Structural Motifs. Journal of the American Chemical Society, 2000, 122, 8265-8270.	6.6	102
7	An efficient approach to calculation of zero-flux atomic surfaces and generation of atomic integration data. Journal of Computational Chemistry, 1995, 16, 1394-1404.	1.5	101
8	Electronic Structures and Energetics of [5,5] and [9,0] Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2002, 124, 8485-8489.	6.6	95
9	Energetics and Site Specificity of the Homolytic Câ^'H Bond Cleavage in Benzenoid Hydrocarbons:Â An ab Initio Electronic Structure Study. Journal of the American Chemical Society, 1996, 118, 5261-5264.	6.6	94
10	Electron flow and electronegativity equalization in the process of bond formation. Journal of Chemical Physics, 1993, 99, 5151-5162.	1.2	91
11	Variational determination of the zero-flux surfaces of atoms in molecules. Molecular Physics, 1995, 84, 707-716.	0.8	80
12	Constraints upon natural spin orbital functionals imposed by properties of a homogeneous electron gas. Journal of Chemical Physics, 1999, 111, 3396-3400.	1.2	77
13	Ionization potentials and electron affinities from the extended Koopmansâ€™ theorem applied to energy-derivative density matrices: The EKTMPn and EKTQCISD methods. Journal of Chemical Physics, 1997, 107, 6804-6811.	1.2	71
14	Endohedral chemical shifts in higher fullerenes with 72-86 carbon atoms. Theoretical Chemistry Accounts, 2001, 106, 364-368.	0.5	67
15	Ionization potentials from the extended Koopmansâ€™ theorem applied to density matrix functional theory. Chemical Physics Letters, 2005, 412, 71-75.	1.2	61
16	Systematic construction of approximate one-matrix functionals for the electron-electron repulsion energy. Journal of Chemical Physics, 2002, 117, 9560-9566.	1.2	46
17	Endohedral effect in inclusion complexes of the C60 cluster. Journal of Chemical Physics, 1992, 96, 8354-8362.	1.2	43
18	On the exactness of simple natural spin-orbital functionals for a high-density homogeneous electron gas. Physical Review B, 2001, 63, .	1.1	39

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19	Approximate one-matrix functionals for the electronâ€“electron repulsion energy from geminal theories. Journal of Chemical Physics, 2003, 119, 6443-6447.	1.2	39
20	Electron intracule densities and Coulomb holes from energy-derivative two-electron reduced density matrices. Journal of Chemical Physics, 1998, 109, 8225-8231.	1.2	38
21	Phase dilemma in density matrix functional theory. Journal of Chemical Physics, 2004, 120, 5987-5992.	1.2	36
22	Topology of electronâ€“electron interactions in atoms and molecules. I. The Hartreeâ€“Fock approximation. Journal of Chemical Physics, 1996, 105, 8187-8194.	1.2	34
23	Description of a homogeneous electron gas with simple functionals of the one-particle density matrix. Physical Review A, 2000, 61, .	1.0	34
24	The atomic softness matrix. Journal of Chemical Physics, 1994, 101, 366-370.	1.2	32
25	Topology of electron-electron interactions in atoms and molecules. II. The correlation cage. Journal of Chemical Physics, 1999, 110, 1882-1887.	1.2	32
26	Response properties and stability conditions in density matrix functional theory. Journal of Chemical Physics, 2001, 115, 5784-5790.	1.2	31
27	Rigorous interpretation of electronic wavefunctions. IV. Origins of the unusual stability of the 1,3-dimethylimidazol-2-ylidene carbene. International Journal of Quantum Chemistry, 1993, 48, 309-319.	1.0	30
28	Density matrix functional theory of weak intermolecular interactions. Journal of Chemical Physics, 2002, 116, 4802.	1.2	30
29	Electronic Structure Studies of 1,2-Didehydrogenation of Arenes and Rearrangement of Arynes to Annelated Cyclopentadienylidenecarbenes. Journal of the American Chemical Society, 1998, 120, 1695-1700.	6.6	29
30	Wigner molecules: The strong-correlation limit of the three-electron harmonium. Journal of Chemical Physics, 2006, 125, 064106.	1.2	29
31	Off-diagonal derivative discontinuities in the reduced density matrices of electronic systems. Journal of Chemical Physics, 2020, 153, 154108.	1.2	29
32	Fast evaluation of electron intracule and extracule densities on large grids of points. Journal of Chemical Physics, 1996, 105, 4151-4158.	1.2	28
33	Approximate one-electron density matrix functionals for the electronâ€“electron repulsion energy from the hypervirial theorem. Journal of Chemical Physics, 1998, 109, 4156-4163.	1.2	28
34	Thermal Rearrangement of Ethynylarenes to Cyclopentafused Polycyclic Aromatic Hydrocarbons:Â An Electronic Structure Study. Journal of the American Chemical Society, 1999, 121, 3773-3778.	6.6	28
35	Robust validation of approximate 1-matrix functionals with few-electron harmonium atoms. Journal of Chemical Physics, 2015, 143, 214101.	1.2	28
36	The three-electron harmonium atom: The lowest-energy doublet and quadruplet states. Journal of Chemical Physics, 2012, 136, 194112.	1.2	27

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37	Benchmark calculations on the lowest-energy singlet, triplet, and quintet states of the four-electron harmonium atom. Journal of Chemical Physics, 2014, 141, 044128.	1.2	26
38	Parameter-free shell model of spherical Coulomb crystals. Physical Review E, 2008, 78, 026416.	0.8	25
39	Nonclassical Aryl Radicals:â€‰ Intermediates or Transition States for the Hydrogen Shift Reactions?. Journal of Organic Chemistry, 1996, 61, 4111-4114.	1.7	24
40	Efficient algorithm for quantitative assessment of similarities among atoms in molecules. Journal of Computational Chemistry, 1996, 17, 1352-1358.	1.5	24
41	Description of a high-density homogeneous electron gas with the Yasuda density matrix functional. Journal of Chemical Physics, 2001, 115, 8725-8730.	1.2	24
42	Strong-correlation limit of four electrons in an isotropic harmonic trap. Physical Review A, 2008, 77, .	1.0	23
43	Variational density matrix functional theory calculations with the lowest-order Yasuda functional. Journal of Chemical Physics, 2002, 117, 67-71.	1.2	22
44	Robust interpolation between weak- and strong-correlation regimes of quantum systems. Journal of Chemical Physics, 2012, 136, 044109.	1.2	22
45	Bulk properties from finiteâ€cluster calculations. VII. Accurate ab initio calculations on the Peierls distortions in polyacene. Journal of Chemical Physics, 1993, 98, 473-477.	1.2	21
46	Wigner molecules: Natural orbitals of strongly correlated two-electron harmonium. Journal of Chemical Physics, 2006, 125, 064105.	1.2	21
47	One-Electron Reduced Density Matrix Functional Theory of Spin-Polarized Systems. Journal of Chemical Theory and Computation, 2020, 16, 1578-1585.	2.3	21
48	Energetics, electronic structures and geometries of didehydroazines. Molecular Physics, 2003, 101, 839-858.	0.8	20
49	New constraints upon the electron-electron repulsion energy functional of the one-electron reduced density matrix. Journal of Chemical Physics, 2005, 123, 164106.	1.2	20
50	Harmonium atoms at weak confinements: The formation of the Wigner molecules. Journal of Chemical Physics, 2017, 146, 044308.	1.2	20
51	Maximum similarity orbitals for analysis of the electronic excited states. International Journal of Quantum Chemistry, 1991, 40, 81-93.	1.0	19
52	Unoccupied natural orbitals in two-electron Coulombic systems. Chemical Physics Letters, 2006, 430, 188-190.	1.2	19
53	Bilinear Constraints upon the Correlation Contribution to the Electronâ€“Electron Repulsion Energy as a Functional of the One-Electron Reduced Density Matrix. Journal of Chemical Theory and Computation, 2019, 15, 4862-4872.	2.3	19
54	A Theory of Molecules: Atoms In Molecules . A Quantum Theory. Richard F. W. Bader. Clarendon (Oxford University Press), New York, 1990. xviii, 438 pp., illus. $120. International Series of Monographs on Chemistry, 22.. Science, 1991, 252, 1566-1567.	6.0	19

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55	Efficient implementation of the Hillerâ€“Sucherâ€“Feinberg identity for the accurate determination of the electron density. Journal of Chemical Physics, 1994, 100, 464-472.	1.2	18
56	Effects of solvation on chemical bonding: An electronâ€flow analysis. Journal of Chemical Physics, 1995, 103, 4967-4974.	1.2	17
57	Benchmark Full Configuration Interaction Calculations on the Lowest-Energy ²P and ⁴P States of the Three-Electron Harmonium Atom. Journal of Chemical Theory and Computation, 2011, 7, 915-920.	2.3	17
58	Electronegativity Equalization in Polyyne Carbon Chains. The Journal of Physical Chemistry, 1996, 100, 6156-6160.	2.9	16
59	Universalities among natural orbitals and occupation numbers pertaining to ground states of two electrons in central potentials. Journal of Chemical Physics, 2019, 151, 184107.	1.2	16
60	Electronic structure of the benzene-tetracyanoethylene complex: A synthesis of molecular orbital and density functional descriptions. International Journal of Quantum Chemistry, 1994, 49, 463-475.	1.0	15
61	The weak-correlation limits of few-electron harmonium atoms. Journal of Chemical Physics, 2013, 139, 224108.	1.2	15
62	Spinâ€“resolved analysis of electronegativity equalization and electron flow in molecules. Journal of Chemical Physics, 1995, 102, 7499-7503.	1.2	14
63	Bulk properties from finite cluster calculations. VIII. Benchmark calculations of the efficiency of extrapolation methods for the HF and MP2 energies of polyacenes. Journal of Computational Chemistry, 1993, 14, 1468-1481.	1.5	13
64	Theoretical thermochemistry of the C60F18, C60F36, and C60F48fluorofullerenes. Molecular Physics, 2001, 99, 1229-1232.	0.8	13
65	Collective natural orbital occupancies of harmonium. Journal of Chemical Physics, 2005, 122, 084102.	1.2	13
66	Size versus volume extensivity of a new class of density matrix functionals. Journal of Chemical Physics, 2004, 120, 10364-10367.	1.2	12
67	Note: The weak-correlation limit of the three-electron harmonium atom. Journal of Chemical Physics, 2011, 134, 116101.	1.2	12
68	Note on the asymptotic isomer count of large fullerenes. Journal of Mathematical Chemistry, 2014, 52, 1-5.	0.7	12
69	Angular-Momentum Extrapolations to the Complete Basis Set Limit: Why and When They Work. Journal of Chemical Theory and Computation, 2021, 17, 3403-3413.	2.3	12
70	A rigorous energy partitioning scheme for analysis of molecular interactions. Molecular Physics, 1995, 85, 121-129.	0.8	11
71	Solitonic natural orbitals. Journal of Chemical Physics, 2018, 148, 134120.	1.2	11
72	From Fredholm to SchrÃ¶dinger via Eikonal: A New Formalism for Revealing Unknown Properties of Natural Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 6918-6933.	2.3	11

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73	Atomic orbitals in molecules. Journal of Chemical Physics, 1998, 108, 4405-4412.	1.2	10
74	Local-density-matrix approximation: Exact asymptotic results for a high-density homogeneous electron gas. Physical Review B, 2005, 71, .	1.1	10
75	Ab InitioCalculations on Large Molecules: Methodology and Applications. Reviews in Computational Chemistry, 2007, , 1-33.	1.5	10
76	Asymptotic equivalence of the shell-model and local-density descriptions of Coulombic systems confined by radially symmetric potentials in two and three dimensions. Journal of Chemical Physics, 2013, 139, 114109.	1.2	10
77	One-electron reduced density matrices of strongly correlated harmonium atoms. Journal of Chemical Physics, 2015, 142, 114104.	1.2	10
78	Partial-wave decomposition of the ground-state wavefunction of the two-electron harmonium atom. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
79	Five- and six-electron harmonium atoms: Highly accurate electronic properties and their application to benchmarking of approximate 1-matrix functionals. Journal of Chemical Physics, 2018, 148, 144107.	1.2	10
80	Natural amplitudes of the ground state of the helium atom: Benchmark calculations and their relevance to the issue of unoccupied natural orbitals in the H2 molecule. Journal of Chemical Physics, 2019, 150, 074111.	1.2	10
81	Shell structures of assemblies of equicharged particles subject to radial power-law confining potentials. Journal of Chemical Physics, 2010, 133, 234902.	1.2	9
82	Natural orbitals of the ground state of the two-electron harmonium atom. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	9
83	Electron correlation contributions to oneâ€electron properties from functionals of the Hartreeâ€“Fock electron density. Journal of Chemical Physics, 1993, 99, 5163-5166.	1.2	8
84	Analytical derivatives of atomic zeroâ€flux surfaces and properties of atoms in molecules with respect to external perturbations. Journal of Chemical Physics, 1996, 105, 8741-8747.	1.2	8
85	Transannular interactions in S82+ and Se82+: Reality or artifact?. International Journal of Quantum Chemistry, 1997, 65, 609-616.	1.0	8
86	Zero-point vibrational energies of spherical Coulomb crystals. Journal of Chemical Physics, 2009, 130, 094902.	1.2	8
87	Shell model of assemblies of equicharged particles subject to radial confining potentials. Journal of Chemical Physics, 2011, 134, 124305.	1.2	8
88	Fullerenes patched by flowers. Open Chemistry, 2013, 11, 527-534.	1.0	8
89	Endohedral motions inside capped single-walled carbon nanotubes. Journal of Chemical Physics, 2003, 118, 4456-4462.	1.2	7
90	Simple approximants for natural orbitals of harmonium. Journal of Chemical Physics, 2005, 123, 234102.	1.2	7

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91	Shell models of two-dimensional Coulomb crystals: Assessment and comparison with the three-dimensional case. Journal of Chemical Physics, 2012, 136, 114306.	1.2	7
92	Accurate electron densities from the Hiller-Sucher-Feinberg identity applied to constrained wavefunctions. Molecular Physics, 1994, 83, 171-181.	0.8	6
93	Properties of Coulomb crystals: Rigorous results. Journal of Chemical Physics, 2008, 128, 164713.	1.2	6
94	Uniform description of the helium isoelectronic series down to the critical nuclear charge with explicitly correlated basis sets derived from regularized Krylov sequences. Journal of Chemical Physics, 2020, 153, 224106.	1.2	6
95	Properties of electron density and other one-electron observables derived from generalized Hillerâ€“Sucherâ€“Feinberg identities. Journal of Chemical Physics, 1998, 109, 1230-1237.	1.2	5
96	Modified Thomson problem. Physical Review E, 2009, 79, 046405.	0.8	5
97	Oscillatory and fluctuating terms in energies of assemblies of equicharged particles subject to spherically symmetric power-law confining potentials. Journal of Chemical Physics, 2013, 139, 104306.	1.2	5
98	Rovibrational states of Wigner molecules in spherically symmetric confining potentials. Journal of Chemical Physics, 2016, 145, 054116.	1.2	5
99	Simpler is often better: Computational efficiency of explicitly correlated two-electron basis sets generated by the regularized Krylov sequences of Nakatsuji. Journal of Chemical Physics, 2018, 149, 184107.	1.2	5
100	The Coulomb, exchange, and correlation components of the electron-electron repulsion in harmonium atoms. Journal of Chemical Physics, 2015, 142, 114105.	1.2	5
101	Construction of explicitly correlated one-electron reduced density matrices. Journal of Chemical Physics, 2020, 153, 224109.	1.2	5
102	Series analysis methods in enumeration of chemical isomers. Theoretica Chimica Acta, 1989, 76, 47-51.	0.9	4
103	Conformations and thermodynamic properties of sulphur homocycles. II. The fluxional S+8radical cation. Molecular Physics, 2002, 100, 1559-1566.	0.8	4
104	Screening-controlled morphologies of Yukawa crystals. Journal of Chemical Physics, 2010, 132, 024708.	1.2	4
105	Electrostatic energy of polygonal charge distributions. Journal of Mathematical Chemistry, 2012, 50, 1378-1385.	0.7	4
106	One-electron densities of freely rotating Wigner molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 235102.	0.6	4
107	Reverse engineering in quantum chemistry: How to reveal the fifthâ€order offâ€diagonal cusp in the oneâ€electron reduced density matrix without actually calculating it. International Journal of Quantum Chemistry, 0, , e26651.	1.0	4
108	Solitonic natural orbitals in Coulombic systems. Journal of Chemical Physics, 2022, 156, 034108.	1.2	4

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109	Systematic analysis of substituent effects. II. Charges and energies of atoms in fluorochloroethanes. International Journal of Quantum Chemistry, 1999, 72, 331-339.	1.0	3
110	Conformations of the S+5and S+6homocyclic radical cations. International Journal of Quantum Chemistry, 2002, 90, 1049-1054.	1.0	3
111	A Theory of Molecules: Atoms In Molecules . A Quantum Theory. Richard F. W. Bader. Clarendon (Oxford University Press), New York, 1990. xviii, 438 pp., illus. $120. International Series of Monographs on Chemistry, 22.. Science, 1991, 252, 1566-1567.	6.0	2
112	First-principles conformational analysis of the C36H36 spheriphane, a prototype hydrocarbon host cage. Journal of Computational Chemistry, 2001, 22, 1279-1286.	1.5	1
113	Electrostatic self-energies of discrete charge distributions on Jordan curves. Journal of Mathematical Chemistry, 2014, 52, 2520-2531.	0.7	1
114	Fullerenes patched by flowers with octagonal core. Open Chemistry, 2014, 12, 90-97.	1.0	1
115	Note: An explicit solution of the optimal superposition and Eckart frame problems. Journal of Chemical Physics, 2016, 145, 026102.	1.2	1
116	Partial-wave decomposition of the one-electron properties of the LiH molecule computed with explicitly correlated basis sets. Molecular Physics, 2022, 120, .	0.8	1
117	A charge granularity correction to electrostatic self-energies of planar charge distributions. Molecular Physics, 2016, 114, 921-927.	0.8	0
118	ERRORS IN APPROXIMATE IONIZATION ENERGIES DUE TO THE ONE-ELECTRON SPACE TRUNCATION OF THE EKT EIGENPROBLEM. Journal of Chemical Physics, 0, , .	1.2	0