

Katarzyna Pernal

List of Publications by Year in descending order

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95
papers

2,782
citations

159585

30
h-index

197818

49
g-index

96
all docs

96
docs citations

96
times ranked

1096
citing authors

#	ARTICLE	IF	CITATIONS
1	An improved density matrix functional by physically motivated repulsive corrections. <i>Journal of Chemical Physics</i> , 2005, 122, 204102.	3.0	176
2	Dispersionless Density Functional Theory. <i>Physical Review Letters</i> , 2009, 103, 263201.	7.8	159
3	Electron localizability indicator for correlated wavefunctions. I. Parallel-spin pairs. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 453-459.	1.4	153
4	The ground state of harmonium. <i>Journal of Chemical Physics</i> , 2000, 113, 8434-8443.	3.0	115
5	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. <i>Journal of Chemical Physics</i> , 2008, 129, 164105.	3.0	98
6	Time-dependent density-matrix-functional theory. <i>Physical Review A</i> , 2007, 75, .	2.5	86
7	Extension of the Hartree-Fock Plus Dispersion Method by First-Order Correlation Effects. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 550-555.	4.6	83
8	Constraints upon natural spin orbital functionals imposed by properties of a homogeneous electron gas. <i>Journal of Chemical Physics</i> , 1999, 111, 3396-3400.	3.0	77
9	Effective Potential for Natural Spin Orbitals. <i>Physical Review Letters</i> , 2005, 94, 233002.	7.8	70
10	Intergeminal Correction to the Antisymmetrized Product of Strongly Orthogonal Geminals Derived from the Extended Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4332-4341.	5.3	66
11	Excitation energies from extended random phase approximation employed with approximate one- and two-electron reduced density matrices. <i>Journal of Chemical Physics</i> , 2012, 137, 204109.	3.0	63
12	Ionization potentials from the extended Koopmans's theorem applied to density matrix functional theory. <i>Chemical Physics Letters</i> , 2005, 412, 71-75.	2.6	61
13	Reduced Density Matrix Functional Theory (RDMFT) and Linear Response Time-Dependent RDMFT (TD-RDMFT). <i>Topics in Current Chemistry</i> , 2015, 368, 125-183.	4.0	61
14	Electron localizability indicator for correlated wavefunctions. II Antiparallel-spin pairs. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 287-293.	1.4	54
15	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. <i>Journal of Chemical Physics</i> , 2009, 130, 114104.	3.0	54
16	The equivalence of the Piris Natural Orbital Functional 5 (PNOF5) and the antisymmetrized product of strongly orthogonal geminal theory. <i>Computational and Theoretical Chemistry</i> , 2013, 1003, 127-129.	2.5	52
17	Electron Correlation from the Adiabatic Connection for Multireference Wave Functions. <i>Physical Review Letters</i> , 2018, 120, 013001.	7.8	49
18	ERPA's APSC: a computationally efficient geminal-based method for accurate description of chemical systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8622-8626.	2.8	48

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19	Systematic construction of approximate one-matrix functionals for the electron-electron repulsion energy. <i>Journal of Chemical Physics</i> , 2002, 117, 9560-9566.	3.0	46
20	Orbital-free effective embedding potential: Density-matrix functional theory case. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2520-2525.	2.0	46
21	Combining density-functional theory and density-matrix-functional theory. <i>Physical Review A</i> , 2010, 82, .	2.5	45
22	Adiabatic approximation of time-dependent density matrix functional response theory. <i>Journal of Chemical Physics</i> , 2007, 127, 214101.	3.0	40
23	On the exactness of simple natural spin-orbital functionals for a high-density homogeneous electron gas. <i>Physical Review B</i> , 2001, 63, .	3.2	39
24	Approximate one-matrix functionals for the electron-electron repulsion energy from geminal theories. <i>Journal of Chemical Physics</i> , 2003, 119, 6443-6447.	3.0	39
25	Correlation Energy from the Adiabatic Connection Formalism for Complete Active Space Wave Functions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3493-3503.	5.3	39
26	Phase dilemma in density matrix functional theory. <i>Journal of Chemical Physics</i> , 2004, 120, 5987-5992.	3.0	36
27	Calculation of electronic excited states of molecules using the Helmholtz free-energy minimum principle. <i>Physical Review A</i> , 2013, 87, .	2.5	35
28	Description of a homogeneous electron gas with simple functionals of the one-particle density matrix. <i>Physical Review A</i> , 2000, 61, .	2.5	34
29	How accurate is the strongly orthogonal geminal theory in predicting excitation energies? Comparison of the extended random phase approximation and the linear response theory approaches. <i>Journal of Chemical Physics</i> , 2014, 140, 014101.	3.0	32
30	Response properties and stability conditions in density matrix functional theory. <i>Journal of Chemical Physics</i> , 2001, 115, 5784-5790.	3.0	31
31	Density matrix functional theory of weak intermolecular interactions. <i>Journal of Chemical Physics</i> , 2002, 116, 4802.	3.0	30
32	Wigner molecules: The strong-correlation limit of the three-electron harmonium. <i>Journal of Chemical Physics</i> , 2006, 125, 064106.	3.0	29
33	Long-range density-matrix-functional theory: Application to a modified homogeneous electron gas. <i>Physical Review A</i> , 2010, 81, .	2.5	29
34	Ensemble density variational methods with self- and ghost-interaction-corrected functionals. <i>Journal of Chemical Physics</i> , 2014, 140, 18A514.	3.0	28
35	Density Matrix Renormalization Group with Dynamical Correlation via Adiabatic Connection. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7575-7585.	5.3	26
36	Description of a high-density homogeneous electron gas with the Yasuda density matrix functional. <i>Journal of Chemical Physics</i> , 2001, 115, 8725-8730.	3.0	24

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37	A minimalistic approach to static and dynamic electron correlations: Amending generalized valence bond method with extended random phase approximation correlation correction. <i>Journal of Chemical Physics</i> , 2016, 144, 244111.	3.0	23
38	On the validity of the extended Koopmans's theorem. <i>Journal of Chemical Physics</i> , 2001, 114, 4359.	3.0	22
39	Variational density matrix functional theory calculations with the lowest-order Yasuda functional. <i>Journal of Chemical Physics</i> , 2002, 117, 67-71.	3.0	22
40	Projected gradient algorithms for Hartree-Fock and density matrix functional theory calculations. <i>Journal of Chemical Physics</i> , 2008, 128, 134108.	3.0	20
41	Excitation energies from range-separated time-dependent density and density matrix functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 184105.	3.0	20
42	Exact and approximate adiabatic connection formulae for the correlation energy in multireference ground and excited states. <i>Journal of Chemical Physics</i> , 2018, 149, 204101.	3.0	20
43	Electronic Excited States from the Adiabatic-Connection Formalism with Complete Active Space Wave Functions. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5534-5538.	4.6	20
44	Unoccupied natural orbitals in two-electron Coulombic systems. <i>Chemical Physics Letters</i> , 2006, 430, 188-190.	2.6	19
45	Coupled-perturbed density-matrix functional theory equations. Application to static polarizabilities. <i>Journal of Chemical Physics</i> , 2006, 124, 014102.	3.0	19
46	Correlation energy from random phase approximations: A reduced density matrices perspective. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25462.	2.0	19
47	Efficient evaluation of electron correlation along the bond-dissociation coordinate in the ground and excited ionic states with dynamic correlation suppression and enhancement functions of the on-top pair density. <i>Physical Review A</i> , 2018, 98, .	2.5	19
48	Open-shell reduced density matrix functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 074104.	3.0	18
49	Structural and Optical Properties of Struvite. Elucidating Structure of Infrared Spectrum in High Frequency Range. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8668-8678.	2.5	18
50	Symmetry-Adapted Perturbation Theory Based on Multiconfigurational Wave Function Description of Monomers. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5538-5555.	5.3	18
51	Second-Order Dispersion Energy Based on Multireference Description of Monomers. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1016-1027.	5.3	17
52	Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5404-5419.	5.3	16
53	Capturing the Dynamic Correlation for Arbitrary Spin-Symmetry CASSCF Reference with Adiabatic Connection Approaches: Insights into the Electronic Structure of the Tetramethyleneethane Diradical. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4668-4674.	4.6	16
54	Frequency-dependent response properties and excitation energies from one-electron density matrix functionals. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5956.	2.8	15

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55	Reduced density matrix embedding. General formalism and inter-domain correlation functional. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21111-21121.	2.8	15
56	Long-range-corrected multiconfiguration density functional with the on-top pair density. <i>Journal of Chemical Physics</i> , 2020, 152, 094102.	3.0	15
57	Interplay between π -Conjugation and Exchange Magnetism in One-Dimensional Porphyrinoid Polymers. <i>Journal of the American Chemical Society</i> , 2022, 144, 12725-12731.	13.7	15
58	Theoretical thermochemistry of the C60F18, C60F36, and C60F48 fluorofullerenes. <i>Molecular Physics</i> , 2001, 99, 1229-1232.	1.7	13
59	Size versus volume extensivity of a new class of density matrix functionals. <i>Journal of Chemical Physics</i> , 2004, 120, 10364-10367.	3.0	12
60	Multiple bond breaking with APSG-based correlation methods: comparison of two approaches. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	12
61	Generalized Valence Bond Perfect-Pairing Made Versatile Through Electron-Pairs Embedding. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4430-4439.	5.3	12
62	Second-Order Exchange-Dispersion Energy Based on a Multireference Description of Monomers. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6712-6723.	5.3	11
63	Reduced Density Matrix-Driven Complete Active Space Self-Consistent Field Corrected for Dynamic Correlation from the Adiabatic Connection. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4351-4360.	5.3	11
64	Efficient Adiabatic Connection Approach for Strongly Correlated Systems: Application to Singlet-Triplet Gaps of Biradicals. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4570-4578.	4.6	11
65	Local-density-matrix approximation: Exact asymptotic results for a high-density homogeneous electron gas. <i>Physical Review B</i> , 2005, 71, .	3.2	10
66	Excitation energies from time-dependent generalized valence bond method. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	10
67	Local Enhancement of Dynamic Correlation in Excited States: Fresh Perspective on Ionicity and Development of Correlation Density Functional Approximation Based on the On-Top Pair Density. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5883-5889.	4.6	10
68	Approximating one-matrix functionals without generalized Pauli constraints. <i>Physical Review A</i> , 2019, 100, .	2.5	9
69	Range-separated multiconfigurational density functional theory methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 0, , e1566.	14.6	9
70	Complete active space and corrected density functional theories helping each other to describe vertical electronic π - π^* excitations in prototype multiple-bonded molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 024111.	3.0	8
71	Electron correlation energy with a combined complete active space and corrected density-functional approach in a small basis versus the reference complete basis set limit: A close agreement. <i>Chemical Physics Letters</i> , 2019, 716, 227-230.	2.6	8
72	How Much Dispersion Energy Is Included in the Multiconfigurational Interaction Energy?. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6280-6293.	5.3	8

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73	Endohedral motions inside capped single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2003, 118, 4456-4462.	3.0	7
74	Molecular interactions in electron-groups embedding generalized valence bond picture. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	7
75	Reproducing benchmark potential energy curves of molecular bond dissociation with small complete active space aided with density and density-matrix functional corrections. <i>Journal of Chemical Physics</i> , 2019, 151, 164122.	3.0	7
76	Excited states in the adiabatic connection fluctuation-dissipation theory: Recovering missing correlation energy from the negative part of the density response spectrum. <i>Journal of Chemical Physics</i> , 2021, 154, 164102.	3.0	7
77	Turning reduced density matrix theory into a practical tool for studying the Mott transition. <i>New Journal of Physics</i> , 2015, 17, 111001.	2.9	6
78	Excitation Energies of Molecules from Ensemble Density Functional Theory. <i>Advances in Quantum Chemistry</i> , 2016, , 199-229.	0.8	6
79	An efficient implementation of time-dependent linear-response theory for strongly orthogonal geminal wave function models. <i>Journal of Chemical Physics</i> , 2022, 156, 174102.	3.0	6
80	A road to a multiconfigurational ensemble density functional theory without ghost interactions. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 880-889.	2.0	5
81	Dispersion Interactions between Molecules in and out of Equilibrium Geometry: Visualization and Analysis. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1312-1319.	2.5	5
82	Third-order dispersion energy from response functions. <i>Journal of Chemical Physics</i> , 2009, 130, 034103.	3.0	4
83	Molecular multibond dissociation with small complete active space augmented by correlation density functionals. <i>Journal of Chemical Physics</i> , 2020, 152, 204118.	3.0	4
84	Dispersion Interactions in Exciton-Localized States. Theory and Applications to π -conjugated and n -conjugated Excited States. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3497-3511.	5.3	4
85	Extension of an Atom-Atom Dispersion Function to Halogen Bonds and Its Use for Rational Design of Drugs and Biocatalysts. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1787-1799.	2.5	3
86	Challenges for large scale simulation: general discussion. <i>Faraday Discussions</i> , 2020, 224, 309-332.	3.2	2
87	Strong correlation in density functional theory: general discussion. <i>Faraday Discussions</i> , 2020, 224, 373-381.	3.2	2
88	New approaches to study excited states in density functional theory: general discussion. <i>Faraday Discussions</i> , 2020, 224, 483-508.	3.2	2
89	Embracing local suppression and enhancement of dynamic correlation effects in a CASiDFT method for efficient description of excited states. <i>Faraday Discussions</i> , 2020, 224, 333-347.	3.2	2
90	Universal on-top description of electron correlation in the ground and excited many-electron states with correlon quasiparticles. <i>Physical Review A</i> , 2020, 102, .	2.5	2

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91	Computer simulation of water and concentrated ionic solutions. Potential fluctuations and electron localization. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2001, 359, 1593-1609.	3.4	1
92	Comment on "Generalization of the Kohn-Sham system that can represent arbitrary one-electron density matrices". Physical Review A, 2017, 96, .	2.5	1
93	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
94	In pursuit of universality. Nature Reviews Chemistry, 2021, 5, 520-521.	30.2	1
95	On-top description of the effect of excitation on electron correlation with quasiparticles. Physical Review A, 2021, 104, .	2.5	0