Katarzyna Pernal

List of Publications by Year in descending order

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	Dispersion Interactions between Molecules in and out of Equilibrium Geometry: Visualization and Analysis. Journal of Physical Chemistry A, 2022, 126, 1312-1319.	2.5	5
2	An efficient implementation of time-dependent linear-response theory for strongly orthogonal geminal wave function models. Journal of Chemical Physics, 2022, 156, 174102.	3.0	6
3	Efficient Adiabatic Connection Approach for Strongly Correlated Systems: Application to Singletâ€“Triplet Gaps of Biradicals. Journal of Physical Chemistry Letters, 2022, 13, 4570-4578.	4.6	11
4	Dispersion Interactions in Exciton-Localized States. Theory and Applications to Ï€â€“Ï€* and nâˆ’Ï€* Excited States. Journal of Chemical Theory and Computation, 2022, 18, 3497-3511.	5.3	4
5	Interplay between Ï€-Conjugation and Exchange Magnetism in One-Dimensional Porphyrinoid Polymers. Journal of the American Chemical Society, 2022, 144, 12725-12731.	13.7	15
6	Extension of an Atomâ€“Atom Dispersion Function to Halogen Bonds and Its Use for Rational Design of Drugs and Biocatalysts. Journal of Physical Chemistry A, 2021, 125, 1787-1799.	2.5	3
7	Excited states in the adiabatic connection fluctuation-dissipation theory: Recovering missing correlation energy from the negative part of the density response spectrum. Journal of Chemical Physics, 2021, 154, 164102.	3.0	7
8	In pursuit of universality. Nature Reviews Chemistry, 2021, 5, 520-521.	30.2	1
9	Symmetry-Adapted Perturbation Theory Based on Multiconfigurational Wave Function Description of Monomers. Journal of Chemical Theory and Computation, 2021, 17, 5538-5555.	5.3	18
10	On-top description of the effect of excitation on electron correlation with quasiparticles. Physical Review A, 2021, 104, .	2.5	0
11	Density Matrix Renormalization Group with Dynamical Correlation via Adiabatic Connection. Journal of Chemical Theory and Computation, 2021, 17, 7575-7585.	5.3	26
12	Structural and Optical Properties of Struvite. Elucidating Structure of Infrared Spectrum in High Frequency Range. Journal of Physical Chemistry A, 2020, 124, 8668-8678.	2.5	18
13	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
14	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
15	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	3.2	2
16	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
17	How Much Dispersion Energy Is Included in the Multiconfigurational Interaction Energy?. Journal of Chemical Theory and Computation, 2020, 16, 6280-6293.	5.3	8
18	Embracing local suppression and enhancement of dynamic correlation effects in a CASÎDFT method for efficient description of excited states. Faraday Discussions, 2020, 224, 333-347.	3.2	2

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19	Universal on-top description of electron correlation in the ground and excited many-electron states with correlon quasiparticles. Physical Review A, 2020, 102, .	2.5	2
20	Reduced Density Matrix-Driven Complete Active Apace Self-Consistent Field Corrected for Dynamic Correlation from the Adiabatic Connection. Journal of Chemical Theory and Computation, 2020, 16, 4351-4360.	5.3	11
21	Long-range-corrected multiconfiguration density functional with the on-top pair density. Journal of Chemical Physics, 2020, 152, 094102.	3.0	15
22	Molecular multibond dissociation with small complete active space augmented by correlation density functionals. Journal of Chemical Physics, 2020, 152, 204118.	3.0	4
23	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. Journal of Physical Chemistry Letters, 2020, 11, 5883-5889.	4.6	10
24	Capturing the Dynamic Correlation for Arbitrary Spin-Symmetry CASSCF Reference with Adiabatic Connection Approaches: Insights into the Electronic Structure of the Tetramethyleneethane Diradical. Journal of Physical Chemistry Letters, 2019, 10, 4668-4674.	4.6	16
25	Approximating one-matrix functionals without generalized Pauli constraints. Physical Review A, 2019, 100, .	2.5	9
26	Generalized Valence Bond Perfect-Pairing Made Versatile Through Electron-Pairs Embedding. Journal of Chemical Theory and Computation, 2019, 15, 4430-4439.	5.3	12
27	Reproducing benchmark potential energy curves of molecular bond dissociation with small complete active space aided with density and density-matrix functional corrections. Journal of Chemical Physics, 2019, 151, 164122.	3.0	7
28	Complete active space and corrected density functional theories helping each other to describe vertical electronic Ï€â€‰â†’â€‰Ï€* excitations in prototype multiple-bonded molecules. Journal of Chemical Physics, 2019, 151, 024111.	3.0	8
29	Second-Order Exchange-Dispersion Energy Based on a Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 6712-6723.	5.3	11
30	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. Chemical Physics Letters, 2019, 716, 227-230.	2.6	8
31	Second-Order Dispersion Energy Based on Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 1016-1027.	5.3	17
32	Electron Correlation from the Adiabatic Connection for Multireference Wave Functions. Physical Review Letters, 2018, 120, 013001.	7.8	49
33	Correlation energy from random phase approximations: A reduced density matrices perspective. International Journal of Quantum Chemistry, 2018, 118, e25462.	2.0	19
34	Molecular interactions in electron-groups embedding generalized valence bond picture. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	7
35	Exact and approximate adiabatic connection formulae for the correlation energy in multireference ground and excited states. Journal of Chemical Physics, 2018, 149, 204101.	3.0	20
36	Multiple bond breaking with APSG-based correlation methods: comparison of two approaches. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12

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37	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. Physical Review A, 2018, 98, .	2.5	19
38	Electronic Excited States from the Adiabatic-Connection Formalism with Complete Active Space Wave Functions. Journal of Physical Chemistry Letters, 2018, 9, 5534-5538.	4.6	20
39	Correlation Energy from the Adiabatic Connection Formalism for Complete Active Space Wave Functions. Journal of Chemical Theory and Computation, 2018, 14, 3493-3503.	5.3	39
40	Comment on â€œGeneralization of the Kohn-Sham system that can represent arbitrary one-electron density matricesâ€• Physical Review A, 2017, 96, .	2.5	1
41	Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. Journal of Chemical Theory and Computation, 2017, 13, 5404-5419.	5.3	16
42	A road to a multiconfigurational ensemble density functional theory without ghost interactions. International Journal of Quantum Chemistry, 2016, 116, 880-889.	2.0	5
43	A minimalistic approach to static and dynamic electron correlations: Amending generalized valence bond method with extended random phase approximation correlation correction. Journal of Chemical Physics, 2016, 144, 244111.	3.0	23
44	Excitation Energies of Molecules from Ensemble Density Functional Theory. Advances in Quantum Chemistry, 2016, , 199-229.	0.8	6
45	Reduced density matrix embedding. General formalism and inter-domain correlation functional. Physical Chemistry Chemical Physics, 2016, 18, 21111-21121.	2.8	15
46	Turning reduced density matrix theory into a practical tool for studying the Mott transition. New Journal of Physics, 2015, 17, 111001.	2.9	6
47	ERPAâ€“APSG: a computationally efficient geminal-based method for accurate description of chemical systems. Physical Chemistry Chemical Physics, 2015, 17, 8622-8626.	2.8	48
48	Reduced Density Matrix Functional Theory (RDMFT) and Linear Response Time-Dependent RDMFT (TD-RDMFT). Topics in Current Chemistry, 2015, 368, 125-183.	4.0	61
49	Excitation energies from time-dependent generalized valence bond method. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
50	Ensemble density variational methods with self- and ghost-interaction-corrected functionals. Journal of Chemical Physics, 2014, 140, 18A514.	3.0	28
51	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. Journal of Chemical Physics, 2014, 140, 014101.	3.0	32
52	Intergeminal Correction to the Antisymmetrized Product of Strongly Orthogonal Geminals Derived from the Extended Random Phase Approximation. Journal of Chemical Theory and Computation, 2014, 10, 4332-4341.	5.3	66
53	Calculation of electronic excited states of molecules using the Helmholtz free-energy minimum principle. Physical Review A, 2013, 87, .	2.5	35
54	The equivalence of the Piris Natural Orbital Functional 5 (PNOF5) and the antisymmetrized product of strongly orthogonal geminal theory. Computational and Theoretical Chemistry, 2013, 1003, 127-129.	2.5	52

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55	Excitation energies from range-separated time-dependent density and density matrix functional theory. Journal of Chemical Physics, 2012, 136, 184105.	3.0	20
56	Excitation energies from extended random phase approximation employed with approximate one- and two-electron reduced density matrices. Journal of Chemical Physics, 2012, 137, 204109.	3.0	63
57	Open-shell reduced density matrix functional theory. Journal of Chemical Physics, 2011, 135, 074104.	3.0	18
58	Combining density-functional theory and density-matrix-functional theory. Physical Review A, 2010, 82, .	2.5	45
59	Extension of the Hartreeâ˜Fock Plus Dispersion Method by First-Order Correlation Effects. Journal of Physical Chemistry Letters, 2010, 1, 550-555.	4.6	83
60	Long-range density-matrix-functional theory: Application to a modified homogeneous electron gas. Physical Review A, 2010, 81, .	2.5	29
61	Third-order dispersion energy from response functions. Journal of Chemical Physics, 2009, 130, 034103.	3.0	4
62	Orbitalâ€free effective embedding potential: Densityâ€matrix functional theory case. International Journal of Quantum Chemistry, 2009, 109, 2520-2525.	2.0	46
63	Dispersionless Density Functional Theory. Physical Review Letters, 2009, 103, 263201.	7.8	159
64	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. Journal of Chemical Physics, 2009, 130, 114104.	3.0	54
65	Projected gradient algorithms for Hartree-Fock and density matrix functional theory calculations. Journal of Chemical Physics, 2008, 128, 134108.	3.0	20
66	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. Journal of Chemical Physics, 2008, 129, 164105.	3.0	98
67	Time-dependent density-matrix-functional theory. Physical Review A, 2007, 75, .	2.5	86
68	Frequency-dependent response properties and excitation energies from one-electron density matrix functionals. Physical Chemistry Chemical Physics, 2007, 9, 5956.	2.8	15
69	Adiabatic approximation of time-dependent density matrix functional response theory. Journal of Chemical Physics, 2007, 127, 214101.	3.0	40
70	Wigner molecules: The strong-correlation limit of the three-electron harmonium. Journal of Chemical Physics, 2006, 125, 064106.	3.0	29
71	Unoccupied natural orbitals in two-electron Coulombic systems. Chemical Physics Letters, 2006, 430, 188-190.	2.6	19
72	Coupled-perturbed density-matrix functional theory equations. Application to static polarizabilities. Journal of Chemical Physics, 2006, 124, 014102.	3.0	19

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73	Ionization potentials from the extended Koopmansâ€™ theorem applied to density matrix functional theory. Chemical Physics Letters, 2005, 412, 71-75.	2.6	61
74	Electron localizability indicator for correlated wavefunctions. II Antiparallel-spin pairs. Theoretical Chemistry Accounts, 2005, 113, 287-293.	1.4	54
75	An improved density matrix functional by physically motivated repulsive corrections. Journal of Chemical Physics, 2005, 122, 204102.	3.0	176
76	Effective Potential for Natural Spin Orbitals. Physical Review Letters, 2005, 94, 233002.	7.8	70
77	Local-density-matrix approximation: Exact asymptotic results for a high-density homogeneous electron gas. Physical Review B, 2005, 71, .	3.2	10
78	Size versus volume extensivity of a new class of density matrix functionals. Journal of Chemical Physics, 2004, 120, 10364-10367.	3.0	12
79	Electron localizability indicator for correlated wavefunctions. I. Parallel-spin pairs. Theoretical Chemistry Accounts, 2004, 112, 453-459.	1.4	153
80	Phase dilemma in density matrix functional theory. Journal of Chemical Physics, 2004, 120, 5987-5992.	3.0	36
81	Endohedral motions inside capped single-walled carbon nanotubes. Journal of Chemical Physics, 2003, 118, 4456-4462.	3.0	7
82	Approximate one-matrix functionals for the electronâ€“electron repulsion energy from geminal theories. Journal of Chemical Physics, 2003, 119, 6443-6447.	3.0	39
83	Systematic construction of approximate one-matrix functionals for the electron-electron repulsion energy. Journal of Chemical Physics, 2002, 117, 9560-9566.	3.0	46
84	Variational density matrix functional theory calculations with the lowest-order Yasuda functional. Journal of Chemical Physics, 2002, 117, 67-71.	3.0	22
85	Density matrix functional theory of weak intermolecular interactions. Journal of Chemical Physics, 2002, 116, 4802.	3.0	30
86	Theoretical thermochemistry of the C60F18, C60F36, and C60F48fluorofullerenes. Molecular Physics, 2001, 99, 1229-1232.	1.7	13
87	On the validity of the extended Koopmansâ€™ theorem. Journal of Chemical Physics, 2001, 114, 4359.	3.0	22
88	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
89	Response properties and stability conditions in density matrix functional theory. Journal of Chemical Physics, 2001, 115, 5784-5790.	3.0	31
90	On the exactness of simple natural spin-orbital functionals for a high-density homogeneous electron gas. Physical Review B, 2001, 63, .	3.2	39

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91	Description of a high-density homogeneous electron gas with the Yasuda density matrix functional. Journal of Chemical Physics, 2001, 115, 8725-8730.	3.0	24
92	Description of a homogeneous electron gas with simple functionals of the one-particle density matrix. Physical Review A, 2000, 61, .	2.5	34
93	The ground state of harmonium. Journal of Chemical Physics, 2000, 113, 8434-8443.	3.0	115
94	Constraints upon natural spin orbital functionals imposed by properties of a homogeneous electron gas. Journal of Chemical Physics, 1999, 111, 3396-3400.	3.0	77
95	Rangeâ€separated multiconfigurational density functional theory methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , e1566.	14.6	9