David A Mazziotti

List of Publications by Year
in descending order

224 papers	7,400 citations	66250 44 h-index	87275 74 g-index
231 all docs	231 docs citations	231 times ranked	2455 citing authors

#	Article	IF	Citations
1	Cooper-pair condensates with nonclassical long-range order on quantum devices. Physical Review Research, 2022, 4, .	1.3	14
2	Relaxation of stationary states on a quantum computer yields a unique spectroscopic fingerprint of the computerâ€™s noise. Communications Physics, 2022, 5, .	2.0	7
3	Simultaneous fermion and exciton condensations from a model Hamiltonian. Physical Review B, 2022, 105, .	1.1	4
4	Resolving correlated states of benzyne with an error-mitigated contracted quantum eigensolver. Physical Review A, 2022, 105, .	1.0	23
5	Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation. Journal of Physical Chemistry Letters, 2022, 13, 1382-1388.	2.1	12
6	Entangled phase of simultaneous fermion and exciton condensations realized. Physical Review B, 2022, 105, .	1.1	5
7	Beginnings of exciton condensation in coronene analog of graphene double layer. Journal of Chemical Physics, 2022, 156, 154702.	1.2	6
8	Elucidating the molecular orbital dependence of the total electronic energy in multireference problems. Journal of Chemical Physics, 2022, 156, .	1.2	2
9	Interplay of Electronic and Geometric Structure Tunes Organic Biradical Character in Bimetallic Tetrathiafulvalene Tetrathiolate Complexes. Journal of Physical Chemistry A, 2022, 126, 3329-3337.	1.1	4
10	Many-fermion simulation from the contracted quantum eigensolver without fermionic encoding of the wave function. Physical Review A, 2022, 105, .	1.0	9
11	Quantum simulation of the Lindblad equationÂusing a unitary decomposition of operators. Physical Review Research, 2022, 4, .	1.3	10
12	Large cumulant eigenvalue as a signature of exciton condensation. Physical Review B, 2022, 105, .	1.1	5
13	Capturing non-Markovian dynamics on near-term quantum computers. Physical Review Research, 2021, 3, .	1.3	44
14	Quantum Solver of Contracted Eigenvalue Equations for Scalable Molecular Simulations on Quantum Computing Devices. Physical Review Letters, 2021, 126, 070504.	2.9	59
15	Accurate singletâ€“triplet gaps in biradicals via the spin averaged anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2021, 154, 134103.	1.2	15
16	Correlation-driven phenomena in periodic molecular systems from variational two-electron reduced density matrix theory. Journal of Chemical Physics, 2021, 154, 214106.	1.2	3
17	Conductance Switching in an Organometallic Single-Electron Transistor Using Current-Constrained Reduced-Density Matrix Theory. Journal of Physical Chemistry A, 2021, 125, 5448-5455.	1.1	2
18	Lowering tomography costs in quantum simulation with a symmetry projected operator basis. Physical Review A, 2021, 103, .	1.0	11

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19	Toward a Resolution of the Static Correlation Problem in Density Functional Theory from Semidefinite Programming. Journal of Physical Chemistry Letters, 2021, 12, 385-391.	2.1	14
20	Exciton Condensation in Molecular-Scale van der Waals Stacks. Journal of Physical Chemistry Letters, 2021, 12, 9906-9911.	2.1	8
21	Quantum simulation of molecules without fermionic encoding of the wave function. New Journal of Physics, 2021, 23, 113037.	1.2	13
22	Quantum-classical hybrid algorithm for the simulation of all-electron correlation. Journal of Chemical Physics, 2021, 155, 244106.	1.2	17
23	Quantum Simulation of Open Quantum Systems Using a Unitary Decomposition of Operators. Physical Review Letters, 2021, 127, 270503.	2.9	47
24	Redox, transmetalation, and stacking properties of tetrathiafulvalene-2,3,6,7-tetrathiolate bridged tin, nickel, and palladium compounds. Chemical Science, 2020, 11, 1066-1078.	3.7	22
25	Non-equilibrium steady state conductivity in cyclo[18]carbon and its boron nitride analogue. Physical Chemistry Chemical Physics, 2020, 22, 23998-24003.	1.3	26
26	Prediction of the Existence of LiCH: A Carbene-like Organometallic Molecule. Journal of Physical Chemistry A, 2020, 124, 9562-9566.	1.1	4
27	Exact two-body expansion of the many-particle wave function. Physical Review A, 2020, 102, .	1.0	15
28	Reversible Switching of Organic Diradical Character via Iron-Based Spin-Crossover. Journal of the American Chemical Society, 2020, 142, 17670-17680.	6.6	30
29	Mapleâ€™s Quantum Chemistry Package in the Chemistry Classroom. Journal of Chemical Education, 2020, 97, 3658-3666.	1.1	8
30	Dual-cone variational calculation of the two-electron reduced density matrix. Physical Review A, 2020, 102, .	1.0	8
31	Active-Space Pair Two-Electron Reduced Density Matrix Theory for Strong Correlation. Journal of Physical Chemistry A, 2020, 124, 4848-4854.	1.1	7
32	Entangled Electrons Drive a Non-superexchange Mechanism in a Cobalt Quinoid Dimer Complex. Journal of Physical Chemistry Letters, 2020, 11, 4584-4590.	2.1	18
33	Potential coexistence of exciton and fermion-pair condensations. Physical Review B, 2020, 101, .	1.1	15
34	Efficient two-electron ansatz for benchmarking quantum chemistry on a quantum computer. Physical Review Research, 2020, 2, .	1.3	13
35	Preparation of an exciton condensate of photons on a 53-qubit quantum computer. Physical Review Research, 2020, 2, .	1.3	29
36	Satisfying fermionic statistics in the modeling of non-Markovian dynamics with one-electron reduced density matrices. Journal of Chemical Physics, 2019, 151, 034111.	1.2	9

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37	Quantum-classical hybrid algorithm using an error-mitigating <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>N</mml:mi></mml:math> -representability condition to compute the Mott metal-insulator transition. Physical Review A, 2019, 100, .	1.0	41
38	Experimental data from a quantum computer verifies the generalized Pauli exclusion principle. Communications Physics, 2019, 2, .	2.0	17
39	Current-constrained one-electron reduced density-matrix theory for non-equilibrium steady-state molecular conductivity. Physical Chemistry Chemical Physics, 2019, 21, 12620-12624.	1.3	4
40	Unraveling the Band Gap Trend in the Narrowest Graphene Nanoribbons from the Spin-Adapted Excited-Spectra Reduced Density Matrix Method. Journal of Physical Chemistry C, 2019, 123, 14619-14624.	1.5	11
41	Sparse non-orthogonal wave function expansions from the extension of the generalized Pauli constraints to the two-electron reduced density matrix. Journal of Chemical Physics, 2019, 150, 144102.	1.2	4
42	Ensemble of Lindblad's trajectories for non-Markovian dynamics. Physical Review A, 2019, 99, .	1.0	14
43	Signature of van der Waals interactions in the cumulant density matrix. Physical Chemistry Chemical Physics, 2019, 21, 23900-23905.	1.3	6
44	Effects of nitrogenous substituent groups on the benzene dication. Molecular Physics, 2018, 116, 1364-1368.	0.8	3
45	Sparsity of the wavefunction from the generalized Pauli exclusion principle. Journal of Chemical Physics, 2018, 148, 054106.	1.2	10
46	Analytical gradients of variational reduced-density-matrix and wavefunction-based methods from an overlap-reweighted semidefinite program. Journal of Chemical Physics, 2018, 149, 164111.	1.2	6
47	Excited-State Spectra of Strongly Correlated Molecules from a Reduced-Density-Matrix Approach. Journal of Physical Chemistry Letters, 2018, 9, 5373-5378.	2.1	14
48	Strong Electron Correlation in Nitrogenase Cofactor, FeMoco. Journal of Physical Chemistry A, 2018, 122, 4988-4996.	1.1	40
49	Current-constrained density-matrix theory to calculate molecular conductivity with increased accuracy. Communications Chemistry, 2018, 1, .	2.0	15
50	Using reduced density matrix techniques to capture static and dynamic correlation in the energy landscape for the decomposition of the CH2CH2ONO radical and support a non-IRC pathway. Journal of Chemical Physics, 2018, 149, 024302.	1.2	6
51	Quantum signature of exciton condensation. Physical Review B, 2018, 98, .	1.1	33
52	Entangling and disentangling many-electron quantum systems with an electric field. Physical Review A, 2018, 97, .	1.0	4
53	Ligand non-innocence and strong correlation in manganese superoxide dismutase mimics. Physical Chemistry Chemical Physics, 2017, 19, 4656-4660.	1.3	18
54	Orbitals, Occupation Numbers, and Band Structure of Short One-Dimensional Cadmium Telluride Polymers. Journal of Physical Chemistry A, 2017, 121, 3142-3147.	1.1	8

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55	Noise-assisted energy transfer from the dilation of the set of one-electron reduced density matrices. Journal of Chemical Physics, 2017, 146, 184101.	1.2	12
56	Pair 2-electron reduced density matrix theory using localized orbitals. Journal of Chemical Physics, 2017, 147, 084101.	1.2	27
57	Analytical nuclear derivatives for the parametric two-electron reduced density matrix method. Chemical Physics Letters, 2017, 685, 300-304.	1.2	5
58	Static and Dynamic Electron Correlation in the Ligand Noninnocent Oxidation of Nickel Dithiolates. Journal of Physical Chemistry A, 2017, 121, 9377-9384.	1.1	17
59	Development and application of a 2-electron reduced density matrix approach to electron transport via molecular junctions. Journal of Chemical Physics, 2017, 147, 184110.	1.2	12
60	Role of the generalized pauli constraints in the quantum chemistry of excited states. International Journal of Quantum Chemistry, 2016, 116, 784-790.	1.0	15
61	Pseudospectral Gaussian quantum dynamics: Efficient sampling of potential energy surfaces. Journal of Chemical Physics, 2016, 144, 164108.	1.2	3
62	Accurate non-adiabatic quantum dynamics from pseudospectral sampling of time-dependent Gaussian basis sets. Journal of Chemical Physics, 2016, 145, 064101.	1.2	5
63	Entangled Electrons Foil Synthesis of Elusive Low-Valent Vanadium Oxo Complex. Journal of Physical Chemistry Letters, 2016, 7, 627-631.	2.1	44
64	Pure-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>N</mml:mi></mml:math>-representability conditions of two-fermion reduced density matrices. Physical Review A, 2016, 94, .	1.0	47
65	Enhanced Constraints for Accurate Lower Bounds on Many-Electron Quantum Energies from Variational Two-Electron Reduced Density Matrix Theory. Physical Review Letters, 2016, 117, 153001.	2.9	50
66	Structure of the oneâ€electron reduced density matrix from the generalized <scp>P</scp>auli exclusion principle. International Journal of Quantum Chemistry, 2015, 115, 1305-1310.	1.0	20
67	Semidefinite programming formulation of linear-scaling electronic structure theories. Physical Review A, 2015, 92, .	1.0	5
68	Large eigenvalue of the cumulant part of the two-electron reduced density matrix as a measure of off-diagonal long-range order. Physical Review A, 2015, 92, .	1.0	21
69	Enhanced computational efficiency in the direct determination of the two-electron reduced density matrix from the anti-Hermitian contracted SchrÃ¶dinger equation with application to ground and excited states of conjugated Ï€-systems. Journal of Chemical Physics, 2015, 143, 134110.	1.2	17
70	Positive semidefinite tensor factorizations of the two-electron integral matrix for low-scaling ab initio electronic structure. Journal of Chemical Physics, 2015, 143, 064103.	1.2	9
71	Communication: Satisfying fermionic statistics in the modeling of open time-dependent quantum systems with one-electron reduced density matrices. Journal of Chemical Physics, 2015, 142, 051102.	1.2	11
72	Strong Electron Correlation in Materials from Pair-Interacting Model Hamiltonians. Journal of Physical Chemistry C, 2015, 119, 14706-14713.	1.5	10

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73	Sufficient condition for the openness of a many-electron quantum system from the violation of a generalized Pauli exclusion principle. Physical Review A, 2015, 91, .	1.0	26
74	Energies and structures in biradical chemistry from the parametric two-electron reduced-density matrix method: applications to the benzene and cyclobutadiene biradicals. Physical Chemistry Chemical Physics, 2015, 17, 12521-12529.	1.3	6
75	Relations between environmental noise and electronic coupling for optimal exciton transfer in one- and two-dimensional homogeneous and inhomogeneous quantum systems. Journal of Chemical Physics, 2014, 141, 224111.	1.2	8
76	Global solutions of Hartree-Fock theory and their consequences for strongly correlated quantum systems. Physical Review A, 2014, 89, .	1.0	16
77	Accurate prediction of diradical chemistry from a single-reference density-matrix method: Model application to the bicyclobutane to gauche-1,3-butadiene isomerization. Journal of Chemical Physics, 2014, 141, 044305.	1.2	3
78	Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules. Physical Review A, 2014, 89, .	1.0	47
79	Molecule-Optimized Basis Sets and Hamiltonians for Accelerated Electronic Structure Calculations of Atoms and Molecules. Journal of Physical Chemistry A, 2014, 118, 495-502.	1.1	2
80	Modulating the Electronic Structure of Chromophores by Chemical Substituents for Efficient Energy Transfer: Application to Fluorone. Journal of Physical Chemistry A, 2014, 118, 6085-6091.	1.1	4
81	Comparison of one-dimensional and quasi-one-dimensional Hubbard models from the variational two-electron reduced-density-matrix method. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	9
82	Global solutions of restricted open-shell Hartree-Fock theory from semidefinite programming with applications to strongly correlated quantum systems. Journal of Chemical Physics, 2014, 140, 124106.	1.2	7
83	Cage versus Prism: Electronic Energies of the Water Hexamer. Journal of Physical Chemistry A, 2013, 117, 6712-6716.	1.1	18
84	Comparison of low-rank tensor expansions for the acceleration of quantum chemistry computations. Journal of Chemical Physics, 2013, 139, 034105.	1.2	6
85	Cumulant reduced density matrices as measures of statistical dependence and entanglement between electronic quantum domains with application to photosynthetic light harvesting. Physical Review A, 2013, 88, .	1.0	24
86	The tensor hypercontracted parametric reduced density matrix algorithm: Coupled-cluster accuracy with O(r4) scaling. Journal of Chemical Physics, 2013, 139, 054110.	1.2	20
87	Relative Energies and Geometries of the cis- and trans-HO₃ Radicals from the Parametric 2-Electron Density Matrix Method. Journal of Physical Chemistry A, 2013, 117, 1817-1825.	1.1	21
88	Theoretical Prediction of the Structures and Energies of Olympicene and its Isomers. Journal of Physical Chemistry A, 2013, 117, 9746-9752.	1.1	33
89	Effect of molecular-orbital rotations on ground-state energies in the parametric two-electron reduced density matrix method. Journal of Chemical Physics, 2013, 138, 244102.	1.2	8
90	Parametric two-electron reduced-density-matrix method with application to diradical rectangular H4. Computational and Theoretical Chemistry, 2013, 1003, 44-49.	1.1	7

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91	Strongly correlated barriers to rotation from parametric two-electron reduced-density-matrix methods in application to the isomerization of diazene. Journal of Chemical Physics, 2012, 136, 034112.	1.2	31
92	Low-rank spectral expansions of two electron excitations for the acceleration of quantum chemistry calculations. Journal of Chemical Physics, 2012, 137, 244103.	1.2	11
93	Effect of strong electron correlation on the efficiency of photosynthetic light harvesting. Journal of Chemical Physics, 2012, 137, 074117.	1.2	23
94	Impact of multichannel and multipole effects on the Cooper minimum in the high-order-harmonic spectrum of argon. Physical Review A, 2012, 85, .	1.0	54
95	Isoelectronic analogue of oxywater: a parametric two-electron reduced-density-matrix study of ammonia oxide. Molecular Physics, 2012, 110, 765-773.	0.8	11
96	Treating molecules in arbitrary spin states using the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2012, 137, 034107.	1.2	6
97	Photoexcited tautomerization of vinyl alcohol to acetylaldehydevia a conical intersection from contracted SchrÃ¶dinger theory. Physical Chemistry Chemical Physics, 2012, 14, 1660-1667.	1.3	12
98	Measurement-driven reconstruction of many-particle quantum processes by semidefinite programming with application to photosynthetic light harvesting. Physical Review A, 2012, 86, .	1.0	17
99	Connection of an elementary class of parametric two-electron reduced-density-matrix methods to the coupled electron-pair approximations. Molecular Physics, 2012, 110, 1917-1925.	0.8	7
100	Significant conditions for the two-electron reduced density matrix from the constructive solution of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>representability. Physical Review A, 2012, 85, .	1.0	20
101	Structure of Fermionic Density Matrices: Complete<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-Representability Conditions. Physical Review Letters, 2012, 108, 263002.	2.9	163
102	Two-Electron Reduced Density Matrix as the Basic Variable in Many-Electron Quantum Chemistry and Physics. Chemical Reviews, 2012, 112, 244-262.	23.0	135
103	Functional Subsystems and Quantum Redundancy in Photosynthetic Light Harvesting. Journal of Physical Chemistry Letters, 2011, 2, 2989-2993.	2.1	42
104	Strong Correlation in Acene Sheets from the Active-Space Variational Two-Electron Reduced Density Matrix Method: Effects of Symmetry and Size. Journal of Physical Chemistry A, 2011, 115, 5632-5640.	1.1	91
105	Conical Intersection of the Ground and First Excited States of Water: Energies and Reduced Density Matrices from the Anti-Hermitian Contracted SchrÃ¶dinger Equation. Journal of Physical Chemistry A, 2011, 115, 14120-14126.	1.1	8
106	Reduced-Density-Matrix Theory for Many-electron Correlation. , 2011, , 61-90.		0
107	Decoherence in Attosecond Photoionization. Physical Review Letters, 2011, 106, 053003.	2.9	99
108	Photoexcited conversion of gauche-1,3-butadiene to bicyclobutane via a conical intersection: Energies and reduced density matrices from the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2011, 135, 024107.	1.2	35

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109	Rank restriction for the variational calculation of two-electron reduced density matrices of many-electron atoms and molecules. Physical Review A, 2011, 84, .	1.0	12
110	Balancing single- and multi-reference correlation in the chemiluminescent reaction of dioxetanone using the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2011, 134, 174110.	1.2	24
111	Populations of Carbonic Acid Isomers at 210 K from a Fast Two-Electron Reduced-Density Matrix Theory. Journal of Physical Chemistry A, 2011, 115, 12011-12016.	1.1	20
112	Large-Scale Semidefinite Programming for Many-Electron Quantum Mechanics. Physical Review Letters, 2011, 106, 083001.	2.9	116
113	Testing the parametric two-electron reduced-density-matrix method with improved functionals: Application to the conversion of hydrogen peroxide to oxywater. Journal of Chemical Physics, 2011, 134, 174102.	1.2	22
114	Strongly correlated mechanisms of a photoexcited radical reaction from the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2011, 134, 034111.	1.2	19
115	Implementation of the time-dependent configuration-interaction singles method for atomic strong-field processes. Physical Review A, 2010, 82, .	1.0	172
116	Isomerization of nitrosomethane to formaldoxime: Energies, geometries, and frequencies from the parametric variational two-electron reduced-density-matrix method. Journal of Chemical Physics, 2010, 133, 034112.	1.2	18
117	Parametrization of the two-electron reduced density matrix for its direct calculation without the many-electron wave function: Generalizations and applications. Physical Review A, 2010, 81, .	1.0	47
118	Exploiting the spatial locality of electron correlation within the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2010, 132, 034110.	1.2	23
119	Energy Barriers of Vinylidene Carbene Reactions from the Anti-Hermitian Contracted SchrÃ¶dinger Equation. Journal of Physical Chemistry A, 2010, 114, 583-588.	1.1	20
120	Strong correlation in hydrogen chains and lattices using the variational two-electron reduced density matrix method. Journal of Chemical Physics, 2010, 133, 014104.	1.2	76
121	Conical intersections in triplet excited states of methylene from the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2010, 132, 154109.	1.2	23
122	Nonequilibrium, steady-state electron transport with N-representable density matrices from the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2010, 132, 104112.	1.2	18
123	Strong electron correlation in the decomposition reaction of dioxetanone with implications for firefly bioluminescence. Journal of Chemical Physics, 2010, 133, 164110.	1.2	71
124	Efficient geometry optimization by Hellmannâ€“Feynman forces with the anti-Hermitian contracted SchrÃ¶dinger equation. Molecular Physics, 2010, 108, 2543-2550.	0.8	3
125	Coupled nuclear and electronic ground-state motion from variational reduced-density-matrix theory with applications to molecules with floppy or resonant hydrogens. Physical Review A, 2009, 79, .	1.0	20
126	Activation energies of sigmatropic shifts in propene and acetone enolate from the anti-Hermitian contracted Schrol̂dinger equation. Journal of Chemical Physics, 2009, 130, 184112.	1.2	28

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127	Convex-set description of quantum phase transitions in the transverse Ising model using reduced-density-matrix theory. Journal of Chemical Physics, 2009, 130, 224102.	1.2	25
128	Direct calculation of excited-state electronic energies and two-electron reduced density matrices from the anti-Hermitian contracted SchrÃ¶dinger equation. Physical Review A, 2009, 80, .	1.0	41
129	Highly multireferenced arynes studied with large active spaces using two-electron reduced density matrices. Journal of Chemical Physics, 2009, 130, 184101.	1.2	33
130	Open-shell energies and two-electron reduced density matrices from the anti-Hermitian contracted SchrÃ¶dinger equation: A spin-coupled approach. Physical Review A, 2009, 80, .	1.0	32
131	Open-shell molecular electronic states from the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2009, 130, 164109.	1.2	18
132	Parametrization of the Two-Electron Reduced Density Matrix for its Direct Calculation without the Many-Electron Wave Function. Physical Review Letters, 2008, 101, 253002.	2.9	72
133	Parametric two-electron reduced-density-matrix method applied to computing molecular energies and properties at nonequilibrium geometries. Journal of Chemical Physics, 2008, 128, 234103.	1.2	32
134	Electronic excited-state energies from a linear response theory based on the ground-state two-electron reduced density matrix. Journal of Chemical Physics, 2008, 128, 114109.	1.2	26
135	Molecular Geometries and Harmonic Frequencies from the Parametric Two-Electron Reduced Density Matrix Method with Application to the HCN â†" HNC Isomerization. Journal of Physical Chemistry B, 2008, 112, 16158-16162.	1.2	32
136	Energy Barriers in the Conversion of Bicyclobutane to gauche-1,3-Butadiene from the Anti-Hermitian Contracted SchrÃ¶dinger Equation. Journal of Physical Chemistry A, 2008, 112, 13684-13690.	1.1	45
137	Active-space two-electron reduced-density-matrix method: Complete active-space calculations without diagonalization of the N-electron Hamiltonian. Journal of Chemical Physics, 2008, 129, 134108.	1.2	161
138	Geminal-based statistics for the energies of many-electron molecular systems. Physical Review A, 2008, 77, .	1.0	3
139	Variational reduced-density-matrix theory applied to the electronic structure of few-electron quantum dots. Physical Review A, 2008, 78, .	1.0	25
140	Cumulant reconstruction of the three-electron reduced density matrix in the anti-Hermitian contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2007, 127, 104104.	1.2	46
141	Global Energy Minima of Molecular Clusters Computed in Polynomial Time with Semidefinite Programming. Physical Review Letters, 2007, 99, 243002.	2.9	8
142	N -Representability. Advances in Chemical Physics, 2007, , 1-9.	0.3	2
143	Natural Orbital Functional Theory. Advances in Chemical Physics, 2007, , 385-427.	0.3	19
144	Contracted SchrÃ¶dinger Equation. Advances in Chemical Physics, 2007, , 165-203.	0.3	6

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145	Entanglement, Electron Correlation, and Density Matrices. Advances in Chemical Physics, 2007, , 493-535.	0.3	35
146	Purification of Correlated Reduced Density Matrices: Review and Applications. Advances in Chemical Physics, 2007, , 205-259.	0.3	4
147	Variational Two-Electron Reduced-Density-Matrix Theory. Advances in Chemical Physics, 2007, , 19-59.	0.3	13
148	Generalized Normal Ordering, Irreducible Brillouin Conditions, and Contracted SchrÃ¶dinger Equations. Advances in Chemical Physics, 2007, , 293-330.	0.3	6
149	Linear Inequalities for Diagonal Elements of Density Matrices. Advances in Chemical Physics, 2007, , 443-483.	0.3	23
150	Theory and Methodology of The Contracted SchrÃ¶dinger Equation. Advances in Chemical Physics, 2007, , 119-164.	0.3	4
151	Canonical Transformation Theory for Dynamic Correlations in Multireference Problems. Advances in Chemical Physics, 2007, , 343-384.	0.3	16
152	Two-electron reduced density matrices from the anti-Hermitian contracted SchrÃ¶dinger equation: Enhanced energies and properties with larger basis sets. Journal of Chemical Physics, 2007, 126, 184101.	1.2	67
153	Multireference many-electron correlation energies from two-electron reduced density matrices computed by solving the anti-Hermitian contracted SchrÃ¶dinger equation. Physical Review A, 2007, 76, .	1.0	77
154	Anti-Hermitian part of the contracted SchrÃ¶dinger equation for the direct calculation of two-electron reduced density matrices. Physical Review A, 2007, 75, .	1.0	101
155	Molecular properties from variational reduced-density-matrix theory with three-particle N-representability conditions. Journal of Chemical Physics, 2007, 126, 024105.	1.2	42
156	Parametric approach to variational two-electron reduced-density-matrix theory. Physical Review A, 2007, 76, .	1.0	44
157	Variational reduced-density-matrix method for ground-state nuclear motion. Physical Review A, 2007, 75, .	1.0	16
158	Determining the Energy Gap between the Cis and Trans Isomers of HO3-Using Geometry Optimization within the Anti-Hermitian Contracted SchrÃ¶dinger and Coupled Cluster Methodsâ€. Journal of Physical Chemistry A, 2007, 111, 12635-12640.	1.1	39
159	Assessing the Efficacy of Nonsteroidal Anti-Inflammatory Drugs Through the Quantum Computation of Molecular Ionization Energies. Journal of Physical Chemistry A, 2007, 111, 7223-7226.	1.1	8
160	Multireference self-consistent-field energies without the many-electron wave function through a variational low-rank two-electron reduced-density-matrix method. Journal of Chemical Physics, 2007, 127, 244105.	1.2	20
161	Cumulants, Extensivity, and the Connected Formulation of the Contracted SchrÃ¶dinger Equation. Advances in Chemical Physics, 2007, , 261-292.	0.3	14
162	Anti-Hermitian Formulation of the Contracted SchrÃ¶dinger Theory. Advances in Chemical Physics, 2007, , 331-342.	0.3	11

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163	Geminal Functional Theory. Advances in Chemical Physics, 2007, , 429-441.	0.3	0
164	Parameterization of the 2-RDM. Advances in Chemical Physics, 2007, , 485-492.	0.3	0
165	The Lower Bound Method for Density Matrices and Semidefinite Programming. Advances in Chemical Physics, 2007, , 61-91.	0.3	10
166	The T 1 and T 2 Representability Conditions. Advances in Chemical Physics, 2007, , 93-101.	0.3	15
167	Semidefinite Programming: Formulations and Primal-Dual Interior-Point Methods. Advances in Chemical Physics, 2007, , 103-118.	0.3	7
168	First-order semidefinite programming for the two-electron treatment of many-electron atoms and molecules. ESAIM: Mathematical Modelling and Numerical Analysis, 2007, 41, 249-259.	0.8	35
169	Recursively generated linear constraints for variational two-particle reduced-density-matrix theory. Chemical Physics Letters, 2007, 445, 79-83.	1.2	6
170	Quantum Chemistry without Wave Functions:â€‰ Two-Electron Reduced Density Matrices. Accounts of Chemical Research, 2006, 39, 207-215.	7.6	106
171	Computation of quantum phase transitions by reduced-density-matrix mechanics. Physical Review A, 2006, 74, .	1.0	41
172	Variational reduced-density-matrix calculations on radicals: An alternative approach to open-shellab initioquantum chemistry. Physical Review A, 2006, 73, .	1.0	23
173	Modeling the influence of a laser pulse on the potential energy surface in optimal molecular control theory. Journal of Chemical Physics, 2006, 124, 234103.	1.2	5
174	Variational Reduced-Density-Matrix Theory Applied to the Potential Energy Surfaces of Carbon Monoxide in the Presence of Electric Fieldsâ€. Journal of Physical Chemistry A, 2006, 110, 5481-5486.	1.1	16
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