David A Mazziotti

List of Publications by Year
in descending order

224 papers	7,400 citations	57758 44 h-index	76900 74 g-index
231 all docs	231 docs citations	231 times ranked	2129 citing authors

#	Article	IF	Citations
1	Contracted Schrödinger equation: Determining quantum energies and two-particle density matrices without wave functions. Physical Review A, 1998, 57, 4219-4234.	2.5	331
2	Approximate solution for electron correlation through the use of Schwinger probes. Chemical Physics Letters, 1998, 289, 419-427.	2.6	261
3	Realization of Quantum Chemistry without Wave Functions through First-Order Semidefinite Programming. Physical Review Letters, 2004, 93, 213001.	7.8	208
4	Anti-Hermitian Contracted Schrödinger Equation: Direct Determination of the Two-Electron Reduced Density Matrices of Many-Electron Molecules. Physical Review Letters, 2006, 97, 143002.	7.8	178
5	Implementation of the time-dependent configuration-interaction singles method for atomic strong-field processes. Physical Review A, 2010, 82, .	2.5	172
6	Uncertainty relations and reduced density matrices: Mapping many-body quantum mechanics onto four particles. Physical Review A, 2001, 63, .	2.5	168
7	Variational minimization of atomic and molecular ground-state energies via the two-particle reduced density matrix. Physical Review A, 2002, 65, .	2.5	164
8	Structure of Fermionic Density Matrices: Complete N-Representability Conditions. Physical Review Letters, 2012, 108, 263002.	7.8	163
9	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.	3.0	161
10	Two-Electron Reduced Density Matrix as the Basic Variable in Many-Electron Quantum Chemistry and Physics. Chemical Reviews, 2012, 112, 244-262.	47.7	135
11	3,5-contracted Schrï¿½dinger equation: Determining quantum energies and reduced density matrices without wave functions. International Journal of Quantum Chemistry, 1998, 70, 557-570.	2.0	126
12	Large-Scale Semidefinite Programming for Many-Electron Quantum Mechanics. Physical Review Letters, 2011, 106, 083001.	7.8	116
13	Variational reduced-density-matrix method using three-particleN-representability conditions with application to many-electron molecules. Physical Review A, 2006, 74, .	2.5	108
14	Pursuit ofN-representability for the contracted Schrödinger equation through density-matrix reconstruction. Physical Review A, 1999, 60, 3618-3626.	2.5	107
15	Quantum Chemistry without Wave Functions:â€‰ Two-Electron Reduced Density Matrices. Accounts of Chemical Research, 2006, 39, 207-215.	15.6	106
16	Anti-Hermitian part of the contracted Schrödinger equation for the direct calculation of two-electron reduced density matrices. Physical Review A, 2007, 75, .	2.5	101
17	Decoherence in Attosecond Photoionization. Physical Review Letters, 2011, 106, 053003.	7.8	99
18	Complete reconstruction of reduced density matrices. Chemical Physics Letters, 2000, 326, 212-218.	2.6	95

#	ARTICLE	IF	CITATIONS
19	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.	2.5	91
20	Variational method for solving the contracted Schrödinger equation through a projection of the N-particle power method onto the two-particle space. Journal of Chemical Physics, 2002, 116, 1239-1249.	3.0	87
21	Comparison of contracted Schrödinger and coupled-cluster theories. Physical Review A, 1999, 60, 4396-4408.	2.5	85
22	First-order semidefinite programming for the direct determination of two-electron reduced density matrices with application to many-electron atoms and molecules. Journal of Chemical Physics, 2004, 121, 10957.	3.0	84
23	Multireference many-electron correlation energies from two-electron reduced density matrices computed by solving the anti-Hermitian contracted Schrödinger equation. Physical Review A, 2007, 76, .	2.5	77
24	Strong correlation in hydrogen chains and lattices using the variational two-electron reduced density matrix method. Journal of Chemical Physics, 2010, 133, 014104.	3.0	76
25	Parametrization of the Two-Electron Reduced Density Matrix for its Direct Calculation without the Many-Electron Wave Function. Physical Review Letters, 2008, 101, 253002.	7.8	72
26	Purification of correlated reduced density matrices. Physical Review E, 2002, 65, 026704.	2.1	71
27	Strong electron correlation in the decomposition reaction of dioxetanone with implications for firefly bioluminescence. Journal of Chemical Physics, 2010, 133, 164110.	3.0	71
28	The cumulant two-particle reduced density matrix as a measure of electron correlation and entanglement. Journal of Chemical Physics, 2006, 125, 174105.	3.0	70
29	Two-electron reduced density matrices from the anti-Hermitian contracted Schrödinger equation: Enhanced energies and properties with larger basis sets. Journal of Chemical Physics, 2007, 126, 184101.	3.0	67
30	Variational two-electron reduced density matrix theory for many-electron atoms and molecules: Implementation of the spin- and symmetry-adapted $T2$ condition through first-order semidefinite programming. Physical Review A, 2005, 72, .	2.5	60
31	Spin and symmetry adaptation of the variational two-electron reduced-density-matrix method. Physical Review A, 2005, 72, .	2.5	59
32	Quantum Solver of Contracted Eigenvalue Equations for Scalable Molecular Simulations on Quantum Computing Devices. Physical Review Letters, 2021, 126, 070504.	7.8	59
33	Impact of multichannel and multipole effects on the Cooper minimum in the high-order-harmonic spectrum of argon. Physical Review A, 2012, 85, .	2.5	54
34	Geminal functional theory: A synthesis of density and density matrix methods. Journal of Chemical Physics, 2000, 112, 10125-10130.	3.0	53
35	Exactness of wave functions from two-body exponential transformations in many-body quantum theory. Physical Review A, 2004, 69, .	2.5	52
36	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.	7.8	50

#	ARTICLE	IF	CITATIONS
37	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, .	2.5	47
38	Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules. Physical Review A, 2014, 89, .	2.5	47
39	Pure-N-representability conditions of two-fermion reduced density matrices. Physical Review A, 2016, 94, .	2.5	47
40	Quantum Simulation of Open Quantum Systems Using a Unitary Decomposition of Operators. Physical Review Letters, 2021, 127, 270503.	7.8	47
41	Solution of the 1,3-contracted Schrödinger equation through positivity conditions on the two-particle reduced density matrix. Physical Review A, 2002, 66, .	2.5	46
42	Cumulant reconstruction of the three-electron reduced density matrix in the anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2007, 127, 104104.	3.0	46
43	Energy Barriers in the Conversion of Bicyclobutane to gauche-1,3-Butadiene from the Anti-Hermitian Contracted Schrödinger Equation. Journal of Physical Chemistry A, 2008, 112, 13684-13690.	2.5	45
44	Parametric approach to variational two-electron reduced-density-matrix theory. Physical Review A, 2007, 76, .	2.5	44
45	Entangled Electrons Foil Synthesis of Elusive Low-Valent Vanadium Oxo Complex. Journal of Physical Chemistry Letters, 2016, 7, 627-631.	4.6	44
46	Capturing non-Markovian dynamics on near-term quantum computers. Physical Review Research, 2021, 3, .	3.6	44
47	Energy functional of the one-particle reduced density matrix: a geminal approach. Chemical Physics Letters, 2001, 338, 323-328.	2.6	43
48	Molecular properties from variational reduced-density-matrix theory with three-particle N-representability conditions. Journal of Chemical Physics, 2007, 126, 024105.	3.0	42
49	Functional Subsystems and Quantum Redundancy in Photosynthetic Light Harvesting. Journal of Physical Chemistry Letters, 2011, 2, 2989-2993.	4.6	42
50	Linear scaling and the 1,2-contracted Schrödinger equation. Journal of Chemical Physics, 2001, 115, 8305-8311.	3.0	41
51	Computation of quantum phase transitions by reduced-density-matrix mechanics. Physical Review A, 2006, 74, .	2.5	41
52	Direct calculation of excited-state electronic energies and two-electron reduced density matrices from the anti-Hermitian contracted Schrödinger equation. Physical Review A, 2009, 80, .	2.5	41
53	Quantum-classical hybrid algorithm using an error-mitigating N-representability condition to compute the Mott metal-insulator transition. Physical Review A, 2019, 100, .	2.5	41
54	Spectral difference methods for solving differential equations. Chemical Physics Letters, 1999, 299, 473-480.	2.6	40

#	Article	IF	Citations
55	Strong Electron Correlation in Nitrogenase Cofactor, FeMoco. Journal of Physical Chemistry A, 2018, 122, 4988-4996.	2.5	40
56	Determining the Energy Gap between the Cis and Trans Isomers of HO3-Using Geometry Optimization within the Anti-Hermitian Contracted Schrödinger and Coupled Cluster Methodsâ€. Journal of Physical Chemistry A, 2007, 111, 12635-12640.	2.5	39
57	Towards idempotent reduced density matrices via particle-hole duality: McWeenyâ€™s purification and beyond. Physical Review E, 2003, 68, 066701.	2.1	38
58	Perturbation theory corrections to the two-particle reduced density matrix variational method. Journal of Chemical Physics, 2004, 121, 1201-1205.	3.0	37
59	Variational two-electron reduced-density-matrix theory: Partial 3-positivity conditions forN-representability. Physical Review A, 2005, 71, .	2.5	37
60	Extraction of electronic excited states from the ground-state two-particle reduced density matrix. Physical Review A, 2003, 68, .	2.5	36
61	Variational reduced-density-matrix calculation of the one-dimensional Hubbard model. Physical Review A, 2006, 73, .	2.5	36
62	Boson correlation energies via variational minimization with the two-particle reduced density matrix: ExactN-representability conditions for harmonic interactions. Physical Review A, 2004, 69, .	2.5	35
63	Entanglement, Electron Correlation, and Density Matrices. Advances in Chemical Physics, 2007, , 493-535.	0.3	35
64	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.	1.9	35
65	Photoexcited conversion of <i>gauche</i>-1,3-butadiene to bicyclobutane via a conical intersection: Energies and reduced density matrices from the anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2011, 135, 024107.	3.0	35
66	Highly multireferenced arynes studied with large active spaces using two-electron reduced density matrices. Journal of Chemical Physics, 2009, 130, 184101.	3.0	33
67	Theoretical Prediction of the Structures and Energies of Olympicene and its Isomers. Journal of Physical Chemistry A, 2013, 117, 9746-9752.	2.5	33
68	Quantum signature of exciton condensation. Physical Review B, 2018, 98, .	3.2	33
69	A propagation toolkit to design quantum controls. Journal of Chemical Physics, 2003, 118, 8168-8172.	3.0	32
70	Parametric two-electron reduced-density-matrix method applied to computing molecular energies and properties at nonequilibrium geometries. Journal of Chemical Physics, 2008, 128, 234103.	3.0	32
71	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.	2.6	32
72	Open-shell energies and two-electron reduced density matrices from the anti-Hermitian contracted Schrödinger equation: A spin-coupled approach. Physical Review A, 2009, 80, .	2.5	32

#	Article	IF	Citations
73	Application of variational reduced-density-matrix theory to the potential energy surfaces of the nitrogen and carbon dimers. Journal of Chemical Physics, 2005, 122, 194104.	3.0	31
74	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.	3.0	31
75	Reversible Switching of Organic Diradical Character via Iron-Based Spin-Crossover. Journal of the American Chemical Society, 2020, 142, 17670-17680.	13.7	30
76	Preparation of an exciton condensate of photons on a 53-qubit quantum computer. Physical Review Research, 2020, 2, .	3.6	29
77	Activation energies of sigmatropic shifts in propene and acetone enolate from the anti-Hermitian contracted Schrolˆdinger equation. Journal of Chemical Physics, 2009, 130, 184112.	3.0	28
78	A general quantum algorithm for open quantum dynamics demonstrated with the Fenna-Matthews-Olson complex. Quantum - the Open Journal for Quantum Science, 0, 6, 726.	0.0	28
79	Comparison of two genres for linear scaling in density functional theory: Purification and density matrix minimization methods. Journal of Chemical Physics, 2005, 122, 084114.	3.0	27
80	Application of variational reduced-density-matrix theory to organic molecules. Journal of Chemical Physics, 2005, 122, 094107.	3.0	27
81	Pair 2-electron reduced density matrix theory using localized orbitals. Journal of Chemical Physics, 2017, 147, 084101.	3.0	27
82	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.	3.0	26
83	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, .	2.5	26
84	Non-equilibrium steady state conductivity in cyclo[18]carbon and its boron nitride analogue. Physical Chemistry Chemical Physics, 2020, 22, 23998-24003.	2.8	26
85	Variational reduced-density-matrix theory applied to the electronic structure of few-electron quantum dots. Physical Review A, 2008, 78, .	2.5	25
86	Convex-set description of quantum phase transitions in the transverse Ising model using reduced-density-matrix theory. Journal of Chemical Physics, 2009, 130, 224102.	3.0	25
87	Balancing single- and multi-reference correlation in the chemiluminescent reaction of dioxetanone using the anti-Hermitian contracted SchrÄ¶dinger equation. Journal of Chemical Physics, 2011, 134, 174110.	3.0	24
88	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, .	2.5	24
89	Variational reduced-density-matrix calculations on radicals: An alternative approach to open-shellab initioquantum chemistry. Physical Review A, 2006, 73, .	2.5	23
90	Linear Inequalities for Diagonal Elements of Density Matrices. Advances in Chemical Physics, 2007, , 443-483.	0.3	23

#	ARTICLE	IF	CITATIONS
91	Exploiting the spatial locality of electron correlation within the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2010, 132, 034110.	3.0	23
92	Conical intersections in triplet excited states of methylene from the anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2010, 132, 154109.	3.0	23
93	Effect of strong electron correlation on the efficiency of photosynthetic light harvesting. Journal of Chemical Physics, 2012, 137, 074117.	3.0	23
94	Resolving correlated states of benzyne with an error-mitigated contracted quantum eigensolver. Physical Review A, 2022, 105, .	2.5	23
95	Spectral difference methods for solving the differential equations of chemical physics. Journal of Chemical Physics, 2002, 117, 2455-2468.	3.0	22
96	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.	3.0	22
97	Redox, transmetalation, and stacking properties of tetrathiafulvalene-2,3,6,7-tetrathiolate bridged tin, nickel, and palladium compounds. Chemical Science, 2020, 11, 1066-1078.	7.4	22
98	Relative Energies and Geometries of the cis- and $trans$-HO_3 Radicals from the Parametric 2-Electron Density Matrix Method. Journal of Physical Chemistry A, 2013, 117, 1817-1825.	2.5	21
99	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, .	2.5	21
100	A Local-Time Algorithm for Achieving Quantum Control. Journal of Physical Chemistry A, 2003, 107, 7264-7268.	2.5	20
101	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.	3.0	20
102	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, .	2.5	20
103	Energy Barriers of Vinylidene Carbene Reactions from the Anti-Hermitian Contracted Schrödinger Equation. Journal of Physical Chemistry A, 2010, 114, 583-588.	2.5	20
104	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.	2.5	20
105	Significant conditions for the two-electron reduced density matrix from the constructive solution of N representability. Physical Review A, 2012, 85, .	2.5	20
106	The tensor hypercontracted parametric reduced density matrix algorithm: Coupled-cluster accuracy with O(r4) scaling. Journal of Chemical Physics, 2013, 139, 054110.	3.0	20
107	Structure of the one-electron reduced density matrix from the generalized Pauli exclusion principle. International Journal of Quantum Chemistry, 2015, 115, 1305-1310.	2.0	20
108	Natural Orbital Functional Theory. Advances in Chemical Physics, 2007, , 385-427.	0.3	19

#	Article	IF	Citations
109	Strongly correlated mechanisms of a photoexcited radical reaction from the anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2011, 134, 034111.	3.0	19
110	Invariance of the cumulant expansion under 1-particle unitary transformations in reduced density matrix theory. Chemical Physics Letters, 2004, 387, 485-489.	2.6	18
111	Open-shell molecular electronic states from the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2009, 130, 164109.	3.0	18
112	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.	3.0	18
113	Nonequilibrium, steady-state electron transport with N-representable density matrices from the anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2010, 132, 104112.	3.0	18
114	Cage versus Prism: Electronic Energies of the Water Hexamer. Journal of Physical Chemistry A, 2013, 117, 6712-6716.	2.5	18
115	Ligand non-innocence and strong correlation in manganese superoxide dismutase mimics. Physical Chemistry Chemical Physics, 2017, 19, 4656-4660.	2.8	18
116	Entangled Electrons Drive a Non-superexchange Mechanism in a Cobalt Quinoid Dimer Complex. Journal of Physical Chemistry Letters, 2020, 11, 4584-4590.	4.6	18
117	Measurement-driven reconstruction of many-particle quantum processes by semidefinite programming with application to photosynthetic light harvesting. Physical Review A, 2012, 86, .	2.5	17
118	Enhanced computational efficiency in the direct determination of the two-electron reduced density matrix from the anti-Hermitian contracted Schrödinger equation with application to ground and excited states of conjugated π-systems. Journal of Chemical Physics, 2015, 143, 134110.	3.0	17
119	Static and Dynamic Electron Correlation in the Ligand Noninnocent Oxidation of Nickel Dithiolates. Journal of Physical Chemistry A, 2017, 121, 9377-9384.	2.5	17
120	Experimental data from a quantum computer verifies the generalized Pauli exclusion principle. Communications Physics, 2019, 2, .	5.3	17
121	Quantum-classical hybrid algorithm for the simulation of all-electron correlation. Journal of Chemical Physics, 2021, 155, 244106.	3.0	17
122	Extraction of ionization energies from the ground-state two-particle reduced density matrix. Chemical Physics Letters, 2004, 400, 90-93.	2.6	16
123	Variational Reduced-Density-Matrix Theory Applied to the Potential Energy Surfaces of Carbon Monoxide in the Presence of Electric Fields†. Journal of Physical Chemistry A, 2006, 110, 5481-5486.	2.5	16
124	Canonical Transformation Theory for Dynamic Correlations in Multireference Problems. Advances in Chemical Physics, 2007, , 343-384.	0.3	16
125	Variational reduced-density-matrix method for ground-state nuclear motion. Physical Review A, 2007, 75, .	2.5	16
126	Global solutions of Hartree-Fock theory and their consequences for strongly correlated quantum systems. Physical Review A, 2014, 89, .	2.5	16

#	ARTICLE	IF	CITATIONS
127	Energy Eigenvalues and Eigenvectors for Bound Quantum Systems Using Parametric Equations of Motion. The Journal of Physical Chemistry, 1995, 99, 112-117.	2.9	15
128	Boson Correlation Energies from Reduced Hamiltonian Interpolation. Physical Review Letters, 1999, 83, 5185-5189.	7.8	15
129	Computation of dipole, quadrupole, and octupole surfaces from the variational two-electron reduced density matrix method. Journal of Chemical Physics, 2006, 125, 144102.	3.0	15
130	The T 1 and T 2 Representability Conditions. Advances in Chemical Physics, 2007, , 93-101.	0.3	15
131	Role of the generalized pauli constraints in the quantum chemistry of excited states. International Journal of Quantum Chemistry, 2016, 116, 784-790.	2.0	15
132	Current-constrained density-matrix theory to calculate molecular conductivity with increased accuracy. Communications Chemistry, 2018, 1, .	4.5	15
133	Exact two-body expansion of the many-particle wave function. Physical Review A, 2020, 102, .	2.5	15
134	Potential coexistence of exciton and fermion-pair condensations. Physical Review B, 2020, 101, .	3.2	15
135	Accurate singlet–triplet gaps in biradicals via the spin averaged anti-Hermitian contracted Schrödinger equation. Journal of Chemical Physics, 2021, 154, 134103.	3.0	15
136	Boson correlation energies and density matrices from reduced Hamiltonian interpolation. Physical Review A, 2000, 62, .	2.5	14
137	Cumulants, Extensivity, and the Connected Formulation of the Contracted Schrödinger Equation. Advances in Chemical Physics, 2007, , 261-292.	0.3	14
138	Excited-State Spectra of Strongly Correlated Molecules from a Reduced-Density-Matrix Approach. Journal of Physical Chemistry Letters, 2018, 9, 5373-5378.	4.6	14
139	Ensemble of Lindblad's trajectories for non-Markovian dynamics. Physical Review A, 2019, 99, .	2.5	14
140	Toward a Resolution of the Static Correlation Problem in Density Functional Theory from Semidefinite Programming. Journal of Physical Chemistry Letters, 2021, 12, 385-391.	4.6	14
141	Cooper-pair condensates with nonclassical long-range order on quantum devices. Physical Review Research, 2022, 4, .	3.6	14
142	Variational Two-Electron Reduced-Density-Matrix Theory. Advances in Chemical Physics, 2007, , 19-59.	0.3	13
143	Efficient two-electron ansatz for benchmarking quantum chemistry on a quantum computer. Physical Review Research, 2020, 2, .	3.6	13
144	Quantum simulation of molecules without fermionic encoding of the wave function. New Journal of Physics, 2021, 23, 113037.	2.9	13

#	Article	IF	Citations
145	Rank restriction for the variational calculation of two-electron reduced density matrices of many-electron atoms and molecules. Physical Review A, 2011, 84, .	2.5	12
146	Photoexcited tautomerization of vinyl alcohol to acetylaldehydevia a conical intersection from contracted Schrödinger theory. Physical Chemistry Chemical Physics, 2012, 14, 1660-1667.	2.8	12
147	Noise-assisted energy transfer from the dilation of the set of one-electron reduced density matrices. Journal of Chemical Physics, 2017, 146, 184101.	3.0	12
148	Development and application of a 2-electron reduced density matrix approach to electron transport via molecular junctions. Journal of Chemical Physics, 2017, 147, 184110.	3.0	12
149	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.	4.6	12
150	Anti-Hermitian Formulation of the Contracted Schrödinger Theory. Advances in Chemical Physics, 2007, , 331-342.	0.3	11
151	Low-rank spectral expansions of two electron excitations for the acceleration of quantum chemistry calculations. Journal of Chemical Physics, 2012, 137, 244103.	3.0	11
152	Isoelectronic analogue of oxywater: a parametric two-electron reduced-density-matrix study of ammonia oxide. Molecular Physics, 2012, 110, 765-773.	1.7	11
153	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.	3.0	11
154	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.	3.1	11
155	Lowering tomography costs in quantum simulation with a symmetry projected operator basis. Physical Review A, 2021, 103, .	2.5	11
156	Trigonometric mapping for the electric field strength in molecular optimal control theory. Chemical Physics Letters, 2005, 416, 142-146.	2.6	10
157	The Lower Bound Method for Density Matrices and Semidefinite Programming. Advances in Chemical Physics, 2007, , 61-91.	0.3	10
158	Strong Electron Correlation in Materials from Pair-Interacting Model Hamiltonians. Journal of Physical Chemistry C, 2015, 119, 14706-14713.	3.1	10
159	Sparsity of the wavefunction from the generalized Pauli exclusion principle. Journal of Chemical Physics, 2018, 148, 054106.	3.0	10
160	Quantum simulation of the Lindblad equationÂusing a unitary decomposition of operators. Physical Review Research, 2022, 4, .	3.6	10
161	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.	1.4	9
162	Positive semidefinite tensor factorizations of the two-electron integral matrix for low-scaling <i>ab initio</i> electronic structure. Journal of Chemical Physics, 2015, 143, 064103.	3.0	9

#	Article	IF	Citations
163	Satisfying fermionic statistics in the modeling of non-Markovian dynamics with one-electron reduced density matrices. Journal of Chemical Physics, 2019, 151, 034111.	3.0	9
164	Many-fermion simulation from the contracted quantum eigensolver without fermionic encoding of the wave function. Physical Review A, 2022, 105, .	2.5	9
165	Spectral difference Lanczos method for efficient time propagation in quantum control theory. Journal of Chemical Physics, 2004, 120, 5962-5967.	3.0	8
166	Variational reduced-density-matrix theory: strength of Hamiltonian-dependent positivity conditions. Chemical Physics Letters, 2004, 398, 434-439.	2.6	8
167	Global Energy Minima of Molecular Clusters Computed in Polynomial Time with Semidefinite Programming. Physical Review Letters, 2007, 99, 243002.	7.8	8
168	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.	2.5	8
169	Conical Intersection of the Ground and First Excited States of Water: Energies and Reduced Density Matrices from the Anti-Hermitian Contracted Schrödinger Equation. Journal of Physical Chemistry A, 2011, 115, 14120-14126.	2.5	8
170	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.	3.0	8
171	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.	3.0	8
172	Orbitals, Occupation Numbers, and Band Structure of Short One-Dimensional Cadmium Telluride Polymers. Journal of Physical Chemistry A, 2017, 121, 3142-3147.	2.5	8
173	Maple's Quantum Chemistry Package in the Chemistry Classroom. Journal of Chemical Education, 2020, 97, 3658-3666.	2.3	8
174	Dual-cone variational calculation of the two-electron reduced density matrix. Physical Review A, 2020, 102, .	2.5	8
175	Exciton Condensation in Molecular-Scale van der Waals Stacks. Journal of Physical Chemistry Letters, 2021, 12, 9906-9911.	4.6	8
176	Semidefinite Programming: Formulations and Primal-Dual Interior-Point Methods. Advances in Chemical Physics, 2007, , 103-118.	0.3	7
177	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.	1.7	7
178	Parametric two-electron reduced-density-matrix method with application to diradical rectangular H4. Computational and Theoretical Chemistry, 2013, 1003, 44-49.	2.5	7
179	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.	3.0	7
180	Active-Space Pair Two-Electron Reduced Density Matrix Theory for Strong Correlation. Journal of Physical Chemistry A, 2020, 124, 4848-4854.	2.5	7

#	Article	IF	Citations
181	Relaxation of stationary states on a quantum computer yields a unique spectroscopic fingerprint of the computer's noise. Communications Physics, 2022, 5, .	5.3	7
182	Comment on "High order finite difference algorithms for solving the Schrödinger equation in molecular dynamics"[J. Chem. Phys. 111, 10827 (1999)]. Journal of Chemical Physics, 2001, 115, 6794-6795.	3.0	6
183	Contracted Schrödinger Equation. Advances in Chemical Physics, 2007, , 165-203.	0.3	6
184	Generalized Normal Ordering, Irreducible Brillouin Conditions, and Contracted Schrödinger Equations. Advances in Chemical Physics, 2007, , 293-330.	0.3	6
185	Recursively generated linear constraints for variational two-particle reduced-density-matrix theory. Chemical Physics Letters, 2007, 445, 79-83.	2.6	6
186	Treating molecules in arbitrary spin states using the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2012, 137, 034107.	3.0	6
187	Comparison of low-rank tensor expansions for the acceleration of quantum chemistry computations. Journal of Chemical Physics, 2013, 139, 034105.	3.0	6
188	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.	2.8	6
189	Highly accurate excited-state energies from direct computation of the 2-electron reduced density matrix by the anti-Hermitian contracted Schrödinger equation. Molecular Physics, 0, , 1-9.	1.7	6
190	Analytical gradients of variational reduced-density-matrix and wavefunction-based methods from an overlap-reweighted semidefinite program. Journal of Chemical Physics, 2018, 149, 164111.	3.0	6
191	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.	3.0	6
192	Signature of van der Waals interactions in the cumulant density matrix. Physical Chemistry Chemical Physics, 2019, 21, 23900-23905.	2.8	6
193	Beginnings of exciton condensation in coronene analog of graphene double layer. Journal of Chemical Physics, 2022, 156, 154702.	3.0	6
194	Modeling the influence of a laser pulse on the potential energy surface in optimal molecular control theory. Journal of Chemical Physics, 2006, 124, 234103.	3.0	5
195	Semidefinite programming formulation of linear-scaling electronic structure theories. Physical Review A, 2015, 92, .	2.5	5
196	Accurate non-adiabatic quantum dynamics from pseudospectral sampling of time-dependent Gaussian basis sets. Journal of Chemical Physics, 2016, 145, 064101.	3.0	5
197	Analytical nuclear derivatives for the parametric two-electron reduced density matrix method. Chemical Physics Letters, 2017, 685, 300-304.	2.6	5
198	Entangled phase of simultaneous fermion and exciton condensations realized. Physical Review B, 2022, 105, .	3.2	5

#	Article	IF	Citations
199	Large cumulant eigenvalue as a signature of exciton condensation. Physical Review B, 2022, 105, .	3.2	5
200	Purification of Correlated Reduced Density Matrices: Review and Applications. Advances in Chemical Physics, 2007, , 205-259.	0.3	4
201	Theory and Methodology of The Contracted Schrödinger Equation. Advances in Chemical Physics, 2007, , 119-164.	0.3	4
202	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.	2.5	4
203	Entangling and disentangling many-electron quantum systems with an electric field. Physical Review A, 2018, 97, .	2.5	4
204	Current-constrained one-electron reduced density-matrix theory for non-equilibrium steady-state molecular conductivity. Physical Chemistry Chemical Physics, 2019, 21, 12620-12624.	2.8	4
205	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.	3.0	4
206	Prediction of the Existence of LiCH: A Carbene-like Organometallic Molecule. Journal of Physical Chemistry A, 2020, 124, 9562-9566.	2.5	4
207	Simultaneous fermion and exciton condensations from a model Hamiltonian. Physical Review B, 2022, 105, .	3.2	4
208	Interplay of Electronic and Geometric Structure Tunes Organic Biradical Character in Bimetallic Tetrathiafulvalene Tetrathiolate Complexes. Journal of Physical Chemistry A, 2022, 126, 3329-3337.	2.5	4
209	Improved perturbative treatment of electronic energies from a minimal-norm approach to many-body perturbation theory. Journal of Chemical Physics, 2005, 122, 124101.	3.0	3
210	Geminal-based statistics for the energies of many-electron molecular systems. Physical Review A, 2008, 77, .	2.5	3
211	Efficient geometry optimization by Hellmann–Feynman forces with the anti-Hermitian contracted Schrödinger equation. Molecular Physics, 2010, 108, 2543-2550.	1.7	3
212	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.	3.0	3
213	Pseudospectral Gaussian quantum dynamics: Efficient sampling of potential energy surfaces. Journal of Chemical Physics, 2016, 144, 164108.	3.0	3
214	Effects of nitrogenous substituent groups on the benzene dication. Molecular Physics, 2018, 116, 1364-1368.	1.7	3
215	Correlation-driven phenomena in periodic molecular systems from variational two-electron reduced density matrix theory. Journal of Chemical Physics, 2021, 154, 214106.	3.0	3
216	N -Representability. Advances in Chemical Physics, 2007, , 1-9.	0.3	2

#	ARTICLE	IF	CITATIONS
217	Molecule-Optimized Basis Sets and Hamiltonians for Accelerated Electronic Structure Calculations of Atoms and Molecules. Journal of Physical Chemistry A, 2014, 118, 495-502.	2.5	2
218	Conductance Switching in an Organometallic Single-Electron Transistor Using Current-Constrained Reduced-Density Matrix Theory. Journal of Physical Chemistry A, 2021, 125, 5448-5455.	2.5	2
219	3,5-contracted Schrödinger equation: Determining quantum energies and reduced density matrices without wave functions. , 1998, 70, 557.		2
220	3,5‑contracted Schrödinger equation: Determining quantum energies and reduced density matrices without wave functions. International Journal of Quantum Chemistry, 1998, 70, 557-570.	2.0	2
221	Elucidating the molecular orbital dependence of the total electronic energy in multireference problems. Journal of Chemical Physics, 2022, 156, .	3.0	2
222	Geminal Functional Theory. Advances in Chemical Physics, 2007, , 429-441.	0.3	0
223	Parameterization of the 2-RDM. Advances in Chemical Physics, 2007, , 485-492.	0.3	0
224	Reduced-Density-Matrix Theory for Many-electron Correlation. , 2011, , 61-90.		0