A Eugene Deprince, Iii

List of Publications by Year
in descending order

51 papers	3,680 citations	279701 23 h-index	189801 50 g-index
56 all docs	56 docs citations	56 times ranked	3521 citing authors

#	Article	IF	Citations
1	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	2.3	961
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
3	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
4	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	23.0	141
5	Accuracy and Efficiency of Coupled-Cluster Theory Using Density Fitting/Cholesky Decomposition, Frozen Natural Orbitals, and a t₁-Transformed Hamiltonian. Journal of Chemical Theory and Computation, 2013, 9, 2687-2696.	2.3	131
6	Selfâ€Assembled Large Au Nanoparticle Arrays with Regular Hot Spots for SERS. Small, 2011, 7, 2365-2371.	5.2	123
7	Large-Scale Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Methods. Journal of Chemical Theory and Computation, 2016, 12, 2260-2271.	2.3	111
8	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
9	Coupled Cluster Theory on Graphics Processing Units I. The Coupled Cluster Doubles Method. Journal of Chemical Theory and Computation, 2011, 7, 1287-1295.	2.3	87
10	Simulation of Near-Edge X-ray Absorption Fine Structure with Time-Dependent Equation-of-Motion Coupled-Cluster Theory. Journal of Physical Chemistry Letters, 2017, 8, 2951-2957.	2.1	83
11	Linear Absorption Spectra from Explicitly Time-Dependent Equation-of-Motion Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2016, 12, 5834-5840.	2.3	77
12	Communication: Resolving the three-body contribution to the lattice energy of crystalline benzene: Benchmark results from coupled-cluster theory. Journal of Chemical Physics, 2014, 140, 121104.	1.2	68
13	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	6.2	66
14	Accurate Noncovalent Interaction Energies Using Truncated Basis Sets Based on Frozen Natural Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 293-299.	2.3	62
15	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
16	Cavity-modulated ionization potentials and electron affinities from quantum electrodynamics coupled-cluster theory. Journal of Chemical Physics, 2021, 154, 094112.	1.2	44
17	Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6617-6624.	2.3	40
18	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

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19	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
20	Radical Dimerization in a Plastic Organic Crystal Leads to Structural and Magnetic Bistability with Wide Thermal Hysteresis. Journal of the American Chemical Society, 2019, 141, 17989-17994.	6.6	31
21	Heterogeneous CPU + GPU Algorithm for Variational Two-Electron Reduced-Density Matrix-Driven Complete Active-Space Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2019, 15, 6164-6178.	2.3	27
22	Emergence of Excited-State Plasmon Modes in Linear Hydrogen Chains from Time-Dependent Quantum Mechanical Methods. Physical Review Letters, 2011, 107, 196806.	2.9	26
23	Accuracy of two-particleN-representability conditions for describing different spin states and the singletâ€"triplet gap in the linear acene series. Molecular Physics, 0, , 1-8.	0.8	25
24	A general time-domain formulation of equation-of-motion coupled-cluster theory for linear spectroscopy. Journal of Chemical Physics, 2019, 151, 204107.	1.2	25
25	Combining Pair-Density Functional Theory and Variational Two-Electron Reduced-Density Matrix Methods. Journal of Chemical Theory and Computation, 2019, 15, 290-302.	2.3	24
26	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
27	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
28	Equation-of-motion cavity quantum electrodynamics coupled-cluster theory for electron attachment. Journal of Chemical Physics, 2022, 156, 054105.	1.2	22
29	Modeling molecule-plasmon interactions using quantized radiation fields within time-dependent electronic structure theory. Journal of Chemical Physics, 2015, 143, 214104.	1.2	21
30	Variational optimization of the two-electron reduced-density matrix under pure-state N-representability conditions. Journal of Chemical Physics, 2016, 145, 164109.	1.2	19
31	Open-shell molecular electronic states from the parametric two-electron reduced-density-matrix method. Journal of Chemical Physics, 2009, 130, 164109.	1.2	18
32	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
33	Diphenylisobenzofuran Bound to Nanocrystalline Metal Oxides: Excimer Formation, Singlet Fission, Electron Injection, and Low Energy Sensitization. Journal of Physical Chemistry C, 2018, 122, 28478-28490.	1.5	18
34	Analytic Energy Gradients for Variational Two-Electron Reduced-Density Matrix Methods within the Density Fitting Approximation. Journal of Chemical Theory and Computation, 2019, 15, 276-289.	2.3	17
35	Plasmonic Amplifiers: Engineering Giant Light Enhancements by Tuning Resonances in Multiscale Plasmonic Nanostructures. Small, 2013, 9, 1939-1946.	5.2	16
36	Global Hybrid Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 2274-2283.	2.3	15

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37	Analytic Energy Gradients for Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4113-4122.	2.3	14
38	Resonance Energy Transfer Mediated by Metalâ€“Dielectric Composite Nanostructures. Journal of Physical Chemistry C, 2018, 122, 18256-18265.	1.5	13
39	Challenges for variational reduced-density-matrix theory with three-particle N-representability conditions. Journal of Chemical Physics, 2021, 155, 174110.	1.2	13
40	N-representability-driven reconstruction of the two-electron reduced-density matrix for a real-time time-dependent electronic structure method. Journal of Chemical Physics, 2014, 141, 214104.	1.2	12
41	Short Iterative Lanczos Integration in Time-Dependent Equation-of-Motion Coupled-Cluster Theory. Journal of Physical Chemistry A, 2021, 125, 5438-5447.	1.1	12
42	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.	2.3	11
43	Orbital angular momentum constraints in the variational optimization of the two-electron reduced-density matrix. Physical Review A, 2019, 100, .	1.0	9
44	Size-extensive seniority-zero energy functionals derived from configuration interaction with double excitations. Journal of Chemical Physics, 2020, 152, 244103.	1.2	9
45	<tt>p</tt> â€ <tt>q</tt> : a tool for prototyping many-body methods for quantum chemistry. Molecular Physics, 2021, 119, .	0.8	9
46	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
47	An adiabatic connection for doubly-occupied configuration interaction wave functions. Journal of Chemical Physics, 2019, 151, 244121.	1.2	5
48	Modeling core-level excitations with variationally optimized reduced-density matrices and the extended random phase approximation. Journal of Chemical Physics, 2018, 149, 234101.	1.2	4
49	Kinetic-energy-based error quantification in Kohnâ€“Sham density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 26492-26501.	1.3	4
50	Spatial and Spin Symmetry Breaking in Semidefinite-Programming-Based Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2018, 14, 2418-2426.	2.3	2
51	A Parametrized Coupled-Pair Functional for Molecular Interactions: PCPF-MI. Journal of Chemical Theory and Computation, 2014, 10, 4324-4331.	2.3	1