Gergely Gidofalvi

List of Publications by Year in descending order

32 papers	2,017 citations	471509 17 h-index	414414 32 g-index
32 all docs	32 docs citations	32 times ranked	1527 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	Representations of Shavitt Graphs Within the Graphical Unitary Group Approach. Journal of Computational Chemistry, 2020, 41, 129-135.	3.3	5
3	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
4	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.	5.3	27
5	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.	5.3	17
6	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.	5.3	14
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.	5.3	111
8	The Representation and Parametrization of Orthogonal Matrices. Journal of Physical Chemistry A, 2015, 119, 7924-7939.	2.5	15
9	The multifacet graphically contracted function method. II. A general procedure for the parameterization of orthogonal matrices and its application to arc factors. Journal of Chemical Physics, 2014, 141, 064106.	3.0	13
10	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
11	Wave function analysis with Shavitt graph density in the graphically contracted function method. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
12	The multifacet graphically contracted function method. I. Formulation and implementation. Journal of Chemical Physics, 2014, 141, 064105.	3.0	29
13	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181.	47.7	559
14	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
15	An efficient recursive algorithm to compute wave function optimization gradients for the graphically contracted function method. International Journal of Quantum Chemistry, 2010, 110, 2938-2948.	2.0	12
16	Exploiting sparsity in the graphically contracted function configuration interaction method. Molecular Physics, 2010, 108, 2717-2724.	1.7	11
17	Computation of determinant expansion coefficients within the graphically contracted function method. Journal of Computational Chemistry, 2009, 30, 2414-2419.	3.3	17
18	The evaluation of spin-density matrices within the graphically contracted function method. International Journal of Quantum Chemistry, 2009, 109, 3552-3563.	2.0	17

#	Article	IF	Citations
19	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, .	2.5	41
20	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
21	Molecular properties from variational reduced-density-matrix theory with three-particle N-representability conditions. Journal of Chemical Physics, 2007, 126, 024105.	3.0	42
22	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
23	Computation of quantum phase transitions by reduced-density-matrix mechanics. Physical Review A, 2006, 74, .	2.5	41
24	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
25	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.	2.5	16
26	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
27	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
28	Application of variational reduced-density-matrix theory to organic molecules. Journal of Chemical Physics, 2005, 122, 094107.	3.0	27
29	Spin and symmetry adaptation of the variational two-electron reduced-density-matrix method. Physical Review A, 2005, 72, .	2.5	59
30	Variational reduced-density-matrix theory: strength of Hamiltonian-dependent positivity conditions. Chemical Physics Letters, 2004, 398, 434-439.	2.6	8
31	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
32	Entropy Loss of Hydroxyl Groups of Balanol upon Binding to Protein Kinase A. Journal of Chemical Education, 2002, 79, 1122.	2.3	5