

Ron Shepard

List of Publications by Year in descending order

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54
papers

4,356
citations

218677

26
h-index

168389

53
g-index

55
all docs

55
docs citations

55
times ranked

2672
citing authors

#	ARTICLE	IF	CITATIONS
1	Spin-density calculation via the graphical unitary group approach. <i>Molecular Physics</i> , 2023, 121, .	1.7	3
2	Wave function analysis with a maximum flow algorithm. <i>Molecular Physics</i> , 2021, 119, e1861351.	1.7	2
3	Representations of Shavitt Graphs Within the Graphical Unitary Group Approach. <i>Journal of Computational Chemistry</i> , 2020, 41, 129-135.	3.3	5
4	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42
5	The all configuration mean energy multiconfiguration self-consistent-field method. I. Equal configuration weights. <i>Molecular Physics</i> , 2019, 117, 2374-2390.	1.7	7
6	The Representation and Parametrization of Orthogonal Matrices. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7924-7939.	2.5	15
7	The multifacet graphically contracted function method. II. A general procedure for the parameterization of orthogonal matrices and its application to arc factors. <i>Journal of Chemical Physics</i> , 2014, 141, 064106.	3.0	13
8	Comparison of multireference configuration interaction potential energy surfaces for H_2O_2 : the effect of internal contraction. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	21
9	Wave function analysis with Shavitt graph density in the graphically contracted function method. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	11
10	The multifacet graphically contracted function method. I. Formulation and implementation. <i>Journal of Chemical Physics</i> , 2014, 141, 064105.	3.0	29
11	The Multiradical Character of One- and Two-Dimensional Graphene Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2581-2584.	13.8	197
12	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. <i>Chemical Reviews</i> , 2012, 112, 108-181.	47.7	559
13	Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules. <i>Advanced Series in Physical Chemistry</i> , 2011, , 415-462.	1.5	18
14	Columbus—a program system for advanced multireference theory calculations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 191-199.	14.6	171
15	An efficient recursive algorithm to compute wave function optimization gradients for the graphically contracted function method. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2938-2948.	2.0	12
16	Exploiting sparsity in the graphically contracted function configuration interaction method. <i>Molecular Physics</i> , 2010, 108, 2717-2724.	1.7	11
17	Computation of determinant expansion coefficients within the graphically contracted function method. <i>Journal of Computational Chemistry</i> , 2009, 30, 2414-2419.	3.3	17
18	The evaluation of spin-density matrices within the graphically contracted function method. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3552-3563.	2.0	17

#	ARTICLE	IF	CITATIONS
19	Evaluation of the Spin-Orbit Interaction within the Graphically Contracted Function Method. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12741-12747.	2.5	9
20	The accuracy of molecular bond lengths computed by multireference electronic structure methods. <i>Chemical Physics</i> , 2008, 349, 37-57.	1.9	27
21	The Multiconfiguration Self-Consistent Field Method. <i>Advances in Chemical Physics</i> , 2007, , 63-200.	0.3	180
22	Some comments on the DIIS method. <i>Molecular Physics</i> , 2007, 105, 2839-2848.	1.7	11
23	Spin-orbit interaction with nonlinear wave functions. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3191-3202.	2.0	10
24	Nonlinear wave function expansions: A progress report. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3203-3218.	2.0	23
25	Hamiltonian Matrix and Reduced Density Matrix Construction with Nonlinear Wave Functions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8880-8892.	2.5	29
26	Optimization of nonlinear wave function parameters. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3190-3207.	2.0	31
27	Computing eigenvalue bounds for iterative subspace matrix methods. <i>Computer Physics Communications</i> , 2005, 167, 90-102.	7.5	9
28	Software for computing eigenvalue bounds for iterative subspace matrix methods. <i>Computer Physics Communications</i> , 2005, 170, 109-114.	7.5	3
29	A General Nonlinear Expansion Form for Electronic Wave Functions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11629-11641.	2.5	44
30	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. <i>Journal of Chemical Physics</i> , 2004, 120, 7330-7339.	3.0	216
31	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. <i>Journal of Chemical Physics</i> , 2004, 120, 7322-7329.	3.0	290
32	Reducing I/O costs for the eigenvalue procedure in large-scale configuration interaction calculations. <i>Journal of Computational Chemistry</i> , 2002, 23, 1121-1125.	3.3	12
33	High-level multireference methods in the quantum-chemistry program system COLUMBUS: Analytic MR-CISD and MR-AQCC gradients and MR-AQCC-LRT for excited states, GUGA spin-orbit CI and parallel CI density. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 664-673.	2.8	401
34	The Subspace Projected Approximate Matrix (SPAM) Modification of the Davidson Method. <i>Journal of Computational Physics</i> , 2001, 172, 472-514.	3.8	11
35	Geometry optimization of excited valence states of formaldehyde using analytical multireference configuration interaction singles and doubles and multireference averaged quadratic coupled-cluster gradients, and the conical intersection formed by the $1^1A'$ and $2^1A'$ states. <i>Journal of Chemical Physics</i> , 2001, 114, 746.	3.0	38
36	A systematic ab initio investigation of the open and ring structures of ozone. <i>Chemical Physics Letters</i> , 1998, 293, 72-80.	2.6	53

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37	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. <i>Journal of Computational Chemistry</i> , 1997, 18, 430-448.	3.3	69
38	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. <i>Journal of Computational Chemistry</i> , 1997, 18, 430-448.	3.3	6
39	THE ANALYTIC GRADIENT METHOD FOR CONFIGURATION INTERACTION WAVE FUNCTIONS. <i>Advanced Series in Physical Chemistry</i> , 1995, , 345-458.	1.5	99
40	An Introduction to GUGA in the Columbus Program System. <i>NATO ASI Series Series B: Physics</i> , 1994, , 447-460.	0.2	7
41	Elimination of the diagonalization bottleneck in parallel Direct-SCF methods. <i>Theoretica Chimica Acta</i> , 1993, 84, 343-351.	0.8	30
42	A parallel implementation of the COLUMBUS multireference configuration interaction program. <i>Theoretica Chimica Acta</i> , 1993, 84, 489-509.	0.8	43
43	The COLUMBUS Standard Integral File Structure: A proposed interchange format. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 865-887.	2.0	3
44	A data compression method applicable to first-order convergent iterative procedures. <i>Journal of Computational Chemistry</i> , 1990, 11, 45-57.	3.3	16
45	A progress report on the status of the COLUMBUSMRCI program system. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 149-165.	2.0	353
46	A general polyatomic potential energy surface fitting method. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 183-198.	2.0	17
47	Geometrical energy derivative evaluation with MRCI wave functions. <i>International Journal of Quantum Chemistry</i> , 1987, 31, 33-44.	2.0	75
48	Search for stationary points on surfaces. <i>The Journal of Physical Chemistry</i> , 1985, 89, 52-57.	2.9	717
49	Multireference configuration interaction treatment of potential energy surfaces: symmetric dissociation of H ₂ O in a double-zeta basis. <i>Chemical Physics Letters</i> , 1984, 105, 363-369.	2.6	68
50	C ₂ V Insertion pathway for BeH ₂ : A test problem for the coupled-cluster single and double excitation model. <i>International Journal of Quantum Chemistry</i> , 1983, 23, 835-845.	2.0	140
51	Theoretical investigation of the $a^1\Sigma^+_u$, $A^1\Sigma^+_u$, $c^3\Sigma^+_g$, and $C^1\Sigma^+_g$ potential energy curves of He ₂ and of He*(2^1S , 2^3S)+He scattering. <i>Journal of Chemical Physics</i> , 1983, 78, 6190-6202.	3.0	72
52	Quantum chemical calculations using the floating point systems, Inc. Model 164 attached processor. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 613-622.	2.0	2
53	New implementation of the graphical unitary group approach for multireference direct configuration interaction calculations. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 91-100.	2.0	68
54	Edge counts for the auxiliary pair graph within the graphical unitary group approach. <i>Molecular Physics</i> , 0, , e1950858.	1.7	1