Ron Shepard

List of Publications by Year
in descending order

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	Search for stationary points on surfaces. The Journal of Physical Chemistry, 1985, 89, 52-57.	2.9	717
2	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181.	47.7	559
3	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 spinâ€“orbit CI and parallel CI density. Physical Chemistry Chemical Physics, 2001, 3, 664-673.	2.8	401
4	A progress report on the status of the COLUMBUSMRCI program system. International Journal of Quantum Chemistry, 1988, 34, 149-165.	2.0	353
5	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. Journal of Chemical Physics, 2004, 120, 7322-7329.	3.0	290
6	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. Journal of Chemical Physics, 2004, 120, 7330-7339.	3.0	216
7	The Multiradical Character of Oneâ€•and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584.	13.8	197
8	The Multiconfiguration Self-Consistent Field Method. Advances in Chemical Physics, 2007, , 63-200.	0.3	180
9	Columbusâ€”a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199.	14.6	171
10	C2V Insertion pathway for BeH2: A test problem for the coupled-cluster single and double excitation model. International Journal of Quantum Chemistry, 1983, 23, 835-845.	2.0	140
11	THE ANALYTIC GRADIENT METHOD FOR CONFIGURATION INTERACTION WAVE FUNCTIONS. Advanced Series in Physical Chemistry, 1995, , 345-458.	1.5	99
12	Geometrical energy derivative evaluation withMRCI wave functions. International Journal of Quantum Chemistry, 1987, 31, 33-44.	2.0	75
13	Theoretical investigation of the aâ€‰3Î£+u, Aâ€‰1Î£+u, câ€‰3Î£+g, and Câ€‰1Î£+g potential energy curves of He2 and of He*(2â€‰1S, 2â€‰3S)+He scattering. Journal of Chemical Physics, 1983, 78, 6190-6202.	3.0	72
14	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. Journal of Computational Chemistry, 1997, 18, 430-448.	3.3	69
15	Multireference configuration interaction treatment of potential energy surfaces: symmetric dissociation of H2O in a double-zeta basis. Chemical Physics Letters, 1984, 105, 363-369.	2.6	68
16	New implementation of the graphical unitary group approach for multireference direct configuration interaction calculations. International Journal of Quantum Chemistry, 1981, 20, 91-100.	2.0	68
17	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	2.6	53
18	A General Nonlinear Expansion Form for Electronic Wave Functionsâ€. Journal of Physical Chemistry A, 2005, 109, 11629-11641.	2.5	44

#	Article	IF	Citations
19	A parallel implementation of the COLUMBUS multireference configuration interaction program. Theoretica Chimica Acta, 1993, 84, 489-509.	0.8	43
20	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
21	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 1â€Š[sup 1]B[sub 1](ïƒ-Ï€[sup â^—]) and 2â€Š[sup 1]A[sub 1](Ï€-Ï€[sup â^—]) states. Journal of Chemical Physics, 2001, 114, 746.	3.0	38
22	Optimization of nonlinear wave function parameters. International Journal of Quantum Chemistry, 2006, 106, 3190-3207.	2.0	31
23	Elimination of the diagonalization bottleneck in parallel Direct-SCF methods. Theoretica Chimica Acta, 1993, 84, 343-351.	0.8	30
24	Hamiltonian Matrix and Reduced Density Matrix Construction with Nonlinear Wave Functions. Journal of Physical Chemistry A, 2006, 110, 8880-8892.	2.5	29
25	The multifacet graphically contracted function method. I. Formulation and implementation. Journal of Chemical Physics, 2014, 141, 064105.	3.0	29
26	The accuracy of molecular bond lengths computed by multireference electronic structure methods. Chemical Physics, 2008, 349, 37-57.	1.9	27
27	Nonlinear wave function expansions: A progress report. International Journal of Quantum Chemistry, 2007, 107, 3203-3218.	2.0	23
28	Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Ââ†'ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	21
29	Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules. Advanced Series in Physical Chemistry, 2011, , 415-462.	1.5	18
30	A general polyatomic potential energy surface fitting method. International Journal of Quantum Chemistry, 1988, 34, 183-198.	2.0	17
31	Computation of determinant expansion coefficients within the graphically contracted function method. Journal of Computational Chemistry, 2009, 30, 2414-2419.	3.3	17
32	The evaluation of spin-density matrices within the graphically contracted function method. International Journal of Quantum Chemistry, 2009, 109, 3552-3563.	2.0	17
33	A data compression method applicable to first-order convergent iterative procedures. Journal of Computational Chemistry, 1990, 11, 45-57.	3.3	16
34	The Representation and Parametrization of Orthogonal Matrices. Journal of Physical Chemistry A, 2015, 119, 7924-7939.	2.5	15
35	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
36	Reducing I/O costs for the eigenvalue procedure in large-scale configuration interaction calculations. Journal of Computational Chemistry, 2002, 23, 1121-1125.	3.3	12

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37	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
38	The Subspace Projected Approximate Matrix (SPAM) Modification of the Davidson Method. Journal of Computational Physics, 2001, 172, 472-514.	3.8	11
39	Some comments on the DIIS method. Molecular Physics, 2007, 105, 2839-2848.	1.7	11
40	Exploiting sparsity in the graphically contracted function configuration interaction method. Molecular Physics, 2010, 108, 2717-2724.	1.7	11
41	Wave function analysis with Shavitt graph density in the graphically contracted function method. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
42	Spinâ€“orbit interaction with nonlinear wave functions. International Journal of Quantum Chemistry, 2007, 107, 3191-3202.	2.0	10
43	Computing eigenvalue bounds for iterative subspace matrix methods. Computer Physics Communications, 2005, 167, 90-102.	7.5	9
44	Evaluation of the Spinâ^'Orbit Interaction within the Graphically Contracted Function Method. Journal of Physical Chemistry A, 2009, 113, 12741-12747.	2.5	9
45	The all configuration mean energy multiconfiguration self-consistent-field method. I. Equal configuration weights. Molecular Physics, 2019, 117, 2374-2390.	1.7	7
46	An Introduction to GUGA in the Columbus Program System. NATO ASI Series Series B: Physics, 1994, , 447-460.	0.2	7
47	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. Journal of Computational Chemistry, 1997, 18, 430-448.	3.3	6
48	Representations of Shavitt Graphs Within the Graphical Unitary Group Approach. Journal of Computational Chemistry, 2020, 41, 129-135.	3.3	5
49	TheCOLUMBUS Standard Integral File Structure: A proposed interchange format. International Journal of Quantum Chemistry, 1991, 40, 865-887.	2.0	3
50	Software for computing eigenvalue bounds for iterative subspace matrix methods. Computer Physics Communications, 2005, 170, 109-114.	7.5	3
51	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	1.7	3
52	Quantum chemical calculations using the floating point systems, Inc. Model 164 attached processor. International Journal of Quantum Chemistry, 1983, 24, 613-622.	2.0	2
53	Wave function analysis with a maximum flow algorithm. Molecular Physics, 2021, 119, e1861351.	1.7	2
54	Edge counts for the auxiliary pair graph within the graphical unitary group approach. Molecular Physics, 0, , e1950858.	1.7	1