Ryan M Richard

List of Publications by Year
in descending order

34 papers	5,725 citations	331670 21 h-index	345221 36 g-index
36 all docs	36 docs citations	36 times ranked	6404 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	<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.	5.3	961
3	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
4	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
5	A generalized many-body expansion and a unified view of fragment-based methods in electronic structure theory. Journal of Chemical Physics, 2012, 137, 064113.	3.0	184
6	Time-Dependent Density-Functional Description of the ¹L_a State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?. Journal of Chemical Theory and Computation, 2011, 7, 1296-1306.	5.3	164
7	Aiming for Benchmark Accuracy with the Many-Body Expansion. Accounts of Chemical Research, 2014, 47, 2828-2836.	15.6	92
8	Understanding the many-body expansion for large systems. I. Precision considerations. Journal of Chemical Physics, 2014, 141, 014108.	3.0	77
9	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit. Journal of Chemical Theory and Computation, 2016, 12, 595-604.	5.3	69
10	Understanding the many-body expansion for large systems. II. Accuracy considerations. Journal of Chemical Physics, 2016, 144, 164105.	3.0	65
11	Many-Body Expansion with Overlapping Fragments: Analysis of Two Approaches. Journal of Chemical Theory and Computation, 2013, 9, 1408-1416.	5.3	57
12	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. Journal of Chemical Theory and Computation, 2016, 12, 627-637.	5.3	56
13	Evaluation of Vapor Pressure and Ultra-High Vacuum Tribological Properties of Ionic Liquids. Tribology Transactions, 2011, 54, 911-919.	2.0	48
14	Periodic boundary conditions for QM/MM calculations: Ewald summation for extended Gaussian basis sets. Journal of Chemical Physics, 2013, 139, 244108.	3.0	42
15	Achieving the CCSD(T) Basis-Set Limit in Sizable Molecular Clusters: Counterpoise Corrections for the Many-Body Expansion. Journal of Physical Chemistry Letters, 2013, 4, 2674-2680.	4.6	40
16	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
17	Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters. Annual Reports in Computational Chemistry, 2013, 9, 25-58.	1.7	37
18	Tribological Testing and Thermal Analysis of an Alkyl Sulfate Series of Ionic Liquids for Use as Aerospace Lubricants. Tribology Transactions, 2012, 55, 815-821.	2.0	32

#	Article	IF	Citations
19	Understanding the Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi. Journal of Chemical Theory and Computation, 2018, 14, 2386-2400.	5.3	32
20	Optimized geometries, vibrational frequencies, and thermochemical properties of mixed boron- and nitrogen-containing three-membered rings. Computational and Theoretical Chemistry, 2007, 806, 113-120.	1.5	28
21	Approaching the complete-basis limit with a truncated many-body expansion. Journal of Chemical Physics, 2013, 139, 224102.	3.0	28
22	Ab initio calculations on the thermodynamic properties of spiropentane and its boron-containing derivatives. Computational and Theoretical Chemistry, 2008, 851, 284-293.	1.5	21
23	G2, G3, and complete basis set calculations of the thermodynamic properties of boron-containing rings: cyclo-CH2BHNH, 1,2-, and 1,3-cyclo-C2H4BHNH. Computational and Theoretical Chemistry, 2006, 776, 89-96.	1.5	18
24	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
25	Density functional calculations on the thermodynamic properties of a series of nitrosocubanes having the formula C8H8â^'x(NO)x (x=1â^'8). Journal of Hazardous Materials, 2009, 164, 1552-1555.	12.4	15
26	B3LYP calculations on the thermodynamic properties of a series of nitroxycubanes having the formula C8H8â^'x(NO3)x (x=1â€“8). Journal of Hazardous Materials, 2009, 164, 1595-1600.	12.4	15
27	Enthalpies of formation of nitrobuckminsterfullerenes: Extrapolation to C60(NO2)60. Computational and Theoretical Chemistry, 2008, 858, 85-87.	1.5	13
28	Ab initio calculations on the thermodynamic properties of azaborospiropentanes. Journal of Molecular Modeling, 2008, 14, 871-878.	1.8	11
29	G2, G3, and complete basis set calculations of optimized geometries, vibrational frequencies, and thermodynamic properties of azatriboretidine and triazaboretidine. Computational and Theoretical Chemistry, 2007, 806, 165-170.	1.5	9
30	G2, G3, and complete basis set calculations on the thermodynamic properties of triazane. Journal of Molecular Modeling, 2008, 14, 29-37.	1.8	9
31	G2, G3, and complete basis set calculations of the thermodynamic properties of aminoborane, diaminoborane, and triaminoborane. Computational and Theoretical Chemistry, 2007, 823, 6-15.	1.5	8
32	B3LYP, G2, G3, and complete basis set calculations of the thermodynamic properties of small cyclic and chain hydroboranes. Computational and Theoretical Chemistry, 2007, 814, 91-98.	1.5	7
33	Ab Initio Calculations on the Thermodynamic Properties of Azaspiropentanes. Journal of Physical Chemistry A, 2008, 112, 2618-2627.	2.5	3
34	G2, G3, and complete basis set calculations of the thermodynamic properties of cis- and trans-triazene. Journal of Molecular Modeling, 2008, 14, 21-27.	1.8	2