

Ryan M Richard

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9209215/publications.pdf>

Version: 2024-02-01

34
papers

5,725
citations

331259

21
h-index

344852

36
g-index

36
all docs

36
docs citations

36
times ranked

6404
citing authors

#	ARTICLE	IF	CITATIONS
1	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021, 121, 4962-4998.	23.0	39
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
3	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	1.2	425
4	Developing a Computational Chemistry Framework for the Exascale Era. <i>Computing in Science and Engineering</i> , 2019, 21, 48-58.	1.2	16
5	Understanding the Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2386-2400.	2.3	32
6	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3185-3197.	2.3	961
7	Understanding the many-body expansion for large systems. II. Accuracy considerations. <i>Journal of Chemical Physics</i> , 2016, 144, 164105.	1.2	65
8	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 595-604.	2.3	69
9	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 627-637.	2.3	56
10	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
11	Understanding the many-body expansion for large systems. I. Precision considerations. <i>Journal of Chemical Physics</i> , 2014, 141, 014108.	1.2	77
12	Aiming for Benchmark Accuracy with the Many-Body Expansion. <i>Accounts of Chemical Research</i> , 2014, 47, 2828-2836.	7.6	92
13	Periodic boundary conditions for QM/MM calculations: Ewald summation for extended Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2013, 139, 244108.	1.2	42
14	Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters. <i>Annual Reports in Computational Chemistry</i> , 2013, 9, 25-58.	0.9	37
15	Many-Body Expansion with Overlapping Fragments: Analysis of Two Approaches. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1408-1416.	2.3	57
16	Achieving the CCSD(T) Basis-Set Limit in Sizable Molecular Clusters: Counterpoise Corrections for the Many-Body Expansion. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2674-2680.	2.1	40
17	Approaching the complete-basis limit with a truncated many-body expansion. <i>Journal of Chemical Physics</i> , 2013, 139, 224102.	1.2	28
18	A generalized many-body expansion and a unified view of fragment-based methods in electronic structure theory. <i>Journal of Chemical Physics</i> , 2012, 137, 064113.	1.2	184

#	ARTICLE	IF	CITATIONS
19	Tribological Testing and Thermal Analysis of an Alkyl Sulfate Series of Ionic Liquids for Use as Aerospace Lubricants. <i>Tribology Transactions</i> , 2012, 55, 815-821.	1.1	32
20	Time-Dependent Density-Functional Description of the π State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1296-1306.	2.3	164
21	Evaluation of Vapor Pressure and Ultra-High Vacuum Tribological Properties of Ionic Liquids. <i>Tribology Transactions</i> , 2011, 54, 911-919.	1.1	48
22	Density functional calculations on the thermodynamic properties of a series of nitrosocubanes having the formula $C_8H_8x(NO)_x$ ($x=1-8$). <i>Journal of Hazardous Materials</i> , 2009, 164, 1552-1555.	6.5	15
23	B3LYP calculations on the thermodynamic properties of a series of nitroxycubanes having the formula $C_8H_8x(NO_3)_x$ ($x=1-8$). <i>Journal of Hazardous Materials</i> , 2009, 164, 1595-1600.	6.5	15
24	G2, G3, and complete basis set calculations on the thermodynamic properties of triazane. <i>Journal of Molecular Modeling</i> , 2008, 14, 29-37.	0.8	9
25	G2, G3, and complete basis set calculations of the thermodynamic properties of cis- and trans-triazene. <i>Journal of Molecular Modeling</i> , 2008, 14, 21-27.	0.8	2
26	Ab initio calculations on the thermodynamic properties of azaborospiropentanes. <i>Journal of Molecular Modeling</i> , 2008, 14, 871-878.	0.8	11
27	Ab initio calculations on the thermodynamic properties of spiropentane and its boron-containing derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 284-293.	1.5	21
28	Enthalpies of formation of nitrobuckminsterfullerenes: Extrapolation to $C_{60}(NO_2)_{60}$. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 85-87.	1.5	13
29	Ab Initio Calculations on the Thermodynamic Properties of Azaspiropentanes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2618-2627.	1.1	3
30	Optimized geometries, vibrational frequencies, and thermochemical properties of mixed boron- and nitrogen-containing three-membered rings. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 113-120.	1.5	28
31	G2, G3, and complete basis set calculations of optimized geometries, vibrational frequencies, and thermodynamic properties of azatriboretidine and triazaboretidine. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 165-170.	1.5	9
32	B3LYP, G2, G3, and complete basis set calculations of the thermodynamic properties of small cyclic and chain hydroboranes. <i>Computational and Theoretical Chemistry</i> , 2007, 814, 91-98.	1.5	7
33	G2, G3, and complete basis set calculations of the thermodynamic properties of aminoborane, diamminoborane, and triaminoborane. <i>Computational and Theoretical Chemistry</i> , 2007, 823, 6-15.	1.5	8
34	G2, G3, and complete basis set calculations of the thermodynamic properties of boron-containing rings: cyclo- CH_2BHNH , 1,2-, and 1,3-cyclo- C_2H_4BHNH . <i>Computational and Theoretical Chemistry</i> , 2006, 776, 89-96.	1.5	18