

Theresa L Windus

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/509685/publications.pdf>

Version: 2024-02-01

63
papers

26,310
citations

361413

20
h-index

149698

56
g-index

65
all docs

65
docs citations

65
times ranked

20580
citing authors

#	ARTICLE	IF	CITATIONS
1	General atomic and molecular electronic structure system. <i>Journal of Computational Chemistry</i> , 1993, 14, 1347-1363.	3.3	19,020
2	Basis Set Exchange: A Community Database for Computational Sciences. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1045-1052.	5.4	2,685
3	6-31G* basis set for atoms K through Zn. <i>Journal of Chemical Physics</i> , 1998, 109, 1223-1229.	3.0	1,766
4	New Basis Set Exchange: An Open, Up-to-Date Resource for the Molecular Sciences Community. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4814-4820.	5.4	1,244
5	High performance computational chemistry: An overview of NWChem a distributed parallel application. <i>Computer Physics Communications</i> , 2000, 128, 260-283.	7.5	698
6	Uncontracted Rys Quadrature Implementation of up to G Functions on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 696-704.	5.3	95
7	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. <i>Journal of Chemical Physics</i> , 2018, 149, 180901.	3.0	72
8	Exascale applications: skin in the game. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2020, 378, 20190056.	3.4	53
9	Valence Virtual Orbitals: An Unambiguous ab Initio Quantification of the LUMO Concept. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10408-10427.	2.5	52
10	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5008-5012.	5.3	47
11	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. <i>Inorganic Chemistry</i> , 2016, 55, 5787-5803.	4.0	46
12	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021, 121, 4962-4998.	47.7	39
13	Accurate ab initio potential energy curves and spectroscopic properties of the four lowest singlet states of C ₂ . <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	37
14	Characterization of Silicon Nanocrystal Surfaces by Multidimensional Solid-State NMR Spectroscopy. <i>Chemistry of Materials</i> , 2017, 29, 10339-10351.	6.7	37
15	Cerium-Catalyzed Hydrosilylation of Acrylates to Give β -Silyl Esters. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 628-631.	13.8	24
16	A Quantum Chemistry Concept Inventory for Physical Chemistry Classes. <i>Journal of Chemical Education</i> , 2016, 93, 605-612.	2.3	23
17	Correlation Energy Extrapolation by Many-Body Expansion. <i>Journal of Physical Chemistry A</i> , 2017, 121, 836-844.	2.5	23
18	O(³ P) + C ₂ H ₄ Potential Energy Surface: Study at the Multireference Level. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12663-12674.	2.5	21

#	ARTICLE	IF	CITATIONS
19	ParFit: A Python-Based Object-Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 391-396.	5.4	21
20	Rationally designed rare earth separation by selective oxalate solubilization. <i>Chemical Communications</i> , 2020, 56, 11386-11389.	4.1	20
21	Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 16327-16341.	8.0	20
22	A Collaborative Informatics Infrastructure for Multi-Scale Science. <i>Cluster Computing</i> , 2005, 8, 243-253.	5.0	18
23	Conformations of Organophosphine Oxides. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8765-8773.	2.5	16
24	Developing a Computational Chemistry Framework for the Exascale Era. <i>Computing in Science and Engineering</i> , 2019, 21, 48-58.	1.2	16
25	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. <i>Journal of Chemical Physics</i> , 2021, 155, 204801.	3.0	15
26	Pinnacle: An approach toward object oriented quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 485-495.	2.0	14
27	Editorial: Modern Architectures and Their Impact on Electronic Structure Theory. <i>Chemical Reviews</i> , 2020, 120, 9015-9020.	47.7	14
28	The transition from the open minimum to the ring minimum on the ground state and on the lowest excited state of like symmetry in ozone: A configuration interaction study. <i>Journal of Chemical Physics</i> , 2016, 144, 104304.	3.0	13
29	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 90-101.	5.3	10
30	Stabilization of X ⁺ Au ⁻ X Complexes on the Au(111) Surface: A Theoretical Investigation and Comparison of X = S, Cl, CH ₃ S, and SiH ₃ S. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3870-3879.	3.1	10
31	Size Dependence of S-bonding on (111) Facets of Cu Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10268-10274.	3.1	9
32	Building capacity for undergraduate education and training in computational molecular science: A collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26359.	2.0	9
33	Projector-Based Quantum Embedding for Molecular Systems: An Investigation of Three Partitioning Approaches. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6384-6393.	2.5	9
34	Load Balancing of Dynamical Nucleation Theory Monte Carlo Simulations through Resource Sharing Barriers. , 2012, , .		8
35	O ⁺ CH ₄ potential energy surface: excited states and biradicals at the multireference level. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	8
36	Cerium-Catalyzed Hydrosilylation of Acrylates to Give β -Silyl Esters. <i>Angewandte Chemie</i> , 2017, 129, 643-646.	2.0	8

#	ARTICLE	IF	CITATIONS
37	Computational Study of the Malonic Acid Tautomerization Products in Highly Concentrated Particles. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2259-2264.	2.5	7
38	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. <i>Parallel Computing</i> , 2021, 108, 102829.	2.1	7
39	Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 158-166.	2.5	6
40	Stability of M3S3 complexes on fcc M(111) surfaces: M = Au, Ag, Cu, and Ni. <i>Surface Science</i> , 2018, 676, 2-8.	1.9	6
41	Rxn Rover: automation of chemical reactions with user-friendly, modular software. <i>Reaction Chemistry and Engineering</i> , 2022, 7, 416-428.	3.7	6
42	Parallel Implementation of the Electronic Structure Code GAMESS. <i>ACS Symposium Series</i> , 1995, , 16-28.	0.5	5
43	O ₂ +C ₂ H ₄ potential energy surface: lowest-lying singlet at the multireference level. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	5
44	Coinage Metal-Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12954-12965.	3.1	5
45	Sulfur adsorption on coinage metal(100) surfaces: propensity for metal-sulfur complex formation relative to (111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26483-26491.	2.8	5
46	POSTER: Utilizing dataflow-based execution for coupled cluster methods. , 2014, , .		4
47	UV-visible spectroscopy of macrocyclic alkyl, nitrosyl and halide complexes of cobalt and rhodium. Experiment and calculation. <i>Dalton Transactions</i> , 2015, 44, 3811-3816.	3.3	4
48	Can ORMAS be used for nonadiabatic coupling calculations? SiCH ₄ and butadiene contours. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	3
49	Computational and NMR Spectroscopic Evidence for Stereochemistry-Dependent Conformations of 2,2,6,6-Tetramethylpiperidiny-Masked 1,2-Diols. <i>Journal of Organic Chemistry</i> , 2015, 80, 9967-9972.	3.2	3
50	Spin-Free [2]R12 Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3176-3184.	5.3	3
51	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Au-S Complex Formation. <i>ChemPhysChem</i> , 2021, 22, 349-358.	2.1	3
52	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. <i>ACS Symposium Series</i> , 0, , 3-53.	0.5	3
53	Applications of Parallel GAMESS. <i>ACS Symposium Series</i> , 1995, , 29-46.	0.5	2
54	A Component Approach to Collaborative Scientific Software Development: Tools and Techniques Utilized by the Quantum Chemistry Science Application Partnership. <i>Scientific Programming</i> , 2008, 16, 287-296.	0.7	2

#	ARTICLE	IF	CITATIONS
55	Saving time and energy with oversubscription and semi-direct M-Åller P-leset second order perturbation methods. <i>Journal of Computational Chemistry</i> , 2017, 38, 830-841.	3.3	2
56	Redox Chemistry of Bis(oxazoliny)cyclopentadienyl and -fluorenyl Rhodium and Iridium Organometallic Compounds. <i>Organometallics</i> , 2018, 37, 4055-4069.	2.3	2
57	Improving efficiency of semi-direct mÅller P-leset second order perturbation methods through oversubscription on multiple nodes. <i>Journal of Computational Chemistry</i> , 2019, 40, 2146-2157.	3.3	2
58	Direct Synthesis of the Phenanthroviridone Skeleton Using a Highly Regioselective Nitroquinone Diels-Alder Reaction. <i>ACS Omega</i> , 2020, 5, 9311-9315.	3.5	2
59	Quantum Mechanical Modeling of Sugar Thermochemistry. <i>ACS Symposium Series</i> , 2010, , 179-199.	0.5	1
60	Rare Earth Elements and Critical Materials: Uses and Availability. <i>ACS Symposium Series</i> , 0, , 63-74.	0.5	1
61	Preface: Mark S. Gordon. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2715-2718.	2.5	0
62	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Au-S Complex Formation. <i>ChemPhysChem</i> , 2021, 22, 343-343.	2.1	0
63	Reversible Ligand Protonation in Noninnocent Constrained-Geometry-Like Group 4 Complexes. <i>Organometallics</i> , 2022, 41, 141-154.	2.3	0