Theresa L Windus

List of Publications by Year
in descending order

63	26,310	361413	149698
papers	citations	20 h-index	56 g-index

65	65	65	20580
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rxn Rover: automation of chemical reactions with user-friendly, modular software. Reaction Chemistry and Engineering, 2022, 7, 416-428.	3.7	6
2	Reversible Ligand Protonation in Noninnocent Constrained-Geometry-Like Group 4 Complexes. Organometallics, 2022, 41, 141-154.	2.3	0
3	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Auâ˜S Complex Formation. ChemPhysChem, 2021, 22, 343-343.	2.1	0
4	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
5	Projector-Based Quantum Embedding for Molecular Systems: An Investigation of Three Partitioning Approaches. Journal of Physical Chemistry A, 2021, 125, 6384-6393.	2.5	9
6	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	2.1	7
7	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Auâ˜S Complex Formation. ChemPhysChem, 2021, 22, 349-358.	2.1	3
8	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
9	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	3.4	53
10	Rationally designed rare earth separation by selective oxalate solubilization. Chemical Communications, 2020, 56, 11386-11389.	4.1	20
11	Editorial: Modern Architectures and Their Impact on Electronic Structure Theory. Chemical Reviews, 2020, 120, 9015-9020.	47.7	14
12	Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. ACS Applied Materials & Interfaces, 2020, 12, 16327-16341.	8.0	20
13	Building capacity for undergraduate education and training in computational molecular science: A collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. International Journal of Quantum Chemistry, 2020, 120, e26359.	2.0	9
14	Direct Synthesis of the Phenanthroviridone Skeleton Using a Highly Regioselective Nitroquinone Dielsâ€“Alder Reaction. ACS Omega, 2020, 5, 9311-9315.	3.5	2
15	New Basis Set Exchange: An Open, Up-to-Date Resource for the Molecular Sciences Community. Journal of Chemical Information and Modeling, 2019, 59, 4814-4820.	5.4	1,244
16	Improving efficiency of semiâ€direct mÃ¸llerâ€“plesset secondâ€order perturbation methods through oversubscription on multiple nodes. Journal of Computational Chemistry, 2019, 40, 2146-2157.	3.3	2
17	Coinage Metalâ€“Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase. Journal of Physical Chemistry C, 2019, 123, 12954-12965.	3.1	5
18	Sulfur adsorption on coinage metal(100) surfaces: propensity for metalâ€“sulfur complex formation relative to (111) surfaces. Physical Chemistry Chemical Physics, 2019, 21, 26483-26491.	2.8	5

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19	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
20	Stability of M3S3 complexes on fcc M(111) surfaces: M = Au, Ag, Cu, and Ni. Surface Science, 2018, 676, 2-8.	1.9	6
21	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	3.0	72
22	Redox Chemistry of Bis(oxazolinyl)cyclopentadienyl and -fluorenyl Rhodium and Iridium Organometallic Compounds. Organometallics, 2018, 37, 4055-4069.	2.3	2
23	Correlation Energy Extrapolation by Many-Body Expansion. Journal of Physical Chemistry A, 2017, 121, 836-844.	2.5	23
24	Computational Study of the Malonic Acid Tautomerization Products in Highly Concentrated Particles. Journal of Physical Chemistry A, 2017, 121, 2259-2264.	2.5	7
25	Saving time and energy with oversubscription and semiâ€direct <scp>M</scp> Ã¸llerâ€“ <scp>P</scp> lesset second order perturbation methods. Journal of Computational Chemistry, 2017, 38, 830-841.	3.3	2
26	ParFit: A Python-Based Object-Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data. Journal of Chemical Information and Modeling, 2017, 57, 391-396.	5.4	21
27	Stabilization of Xâ€“Auâ€“X Complexes on the Au(111) Surface: A Theoretical Investigation and Comparison of X = S, Cl, CH₃S, and SiH₃S. Journal of Physical Chemistry C, 2017, 121, 3870-3879.	3.1	10
28	Preface: Mark S. Gordon. Journal of Physical Chemistry A, 2017, 121, 2715-2718.	2.5	0
29	Ceriumâ€Catalyzed Hydrosilylation of Acrylates to Give Î±â€Silyl Esters. Angewandte Chemie, 2017, 129, 643-646.	2.0	8
30	Ceriumâ€Catalyzed Hydrosilylation of Acrylates to Give Î±â€Silyl Esters. Angewandte Chemie - International Edition, 2017, 56, 628-631.	13.8	24
31	Characterization of Silicon Nanocrystal Surfaces by Multidimensional Solid-State NMR Spectroscopy. Chemistry of Materials, 2017, 29, 10339-10351.	6.7	37
32	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. Journal of Chemical Physics, 2016, 144, 104304.	3.0	13
33	Size Dependence of S-bonding on (111) Facets of Cu Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 10268-10274.	3.1	9
34	Spin-Free [2]_{R12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 3176-3184.	5.3	3
35	A Quantum Chemistry Concept Inventory for Physical Chemistry Classes. Journal of Chemical Education, 2016, 93, 605-612.	2.3	23
36	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. Inorganic Chemistry, 2016, 55, 5787-5803.	4.0	46

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37	UV-visible spectroscopy of macrocyclic alkyl, nitrosyl and halide complexes of cobalt and rhodium. Experiment and calculation. Dalton Transactions, 2015, 44, 3811-3816.	3.3	4
38	Valence Virtual Orbitals: An Unambiguous ab Initio Quantification of the LUMO Concept. Journal of Physical Chemistry A, 2015, 119, 10408-10427.	2.5	52
39	Conformations of Organophosphine Oxides. Journal of Physical Chemistry A, 2015, 119, 8765-8773.	2.5	16
40	Computational and NMR Spectroscopic Evidence for Stereochemistry-Dependent Conformations of 2,2,6,6-Tetramethylpiperidinyl-Masked 1,2-Diols. Journal of Organic Chemistry, 2015, 80, 9967-9972.	3.2	3
41	POSTER: Utilizing dataflow-based execution for coupled cluster methods. , 2014, , .		4
42	Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. Computational and Theoretical Chemistry, 2014, 1040-1041, 158-166.	2.5	6
43	Accurate ab initio potential energy curves and spectroscopic properties of the four lowest singlet states of C2. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	37
44	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. Journal of Chemical Theory and Computation, 2014, 10, 90-101.	5.3	10
45	OÂ+ÂC2H4 potential energy surface: lowest-lying singlet at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
46	Load Balancing of Dynamical Nucleation Theory Monte Carlo Simulations through Resource Sharing Barriers. , 2012, , .		8
47	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. Journal of Chemical Theory and Computation, 2012, 8, 5008-5012.	5.3	47
48	Can ORMAS be used for nonadiabatic coupling calculations? SiCH4 and butadiene contours. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	3
49	OÂ+ÂC2H4 potential energy surface: excited states and biradicals at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	8
50	Quantum Mechanical Modeling of Sugar Thermochemistry. ACS Symposium Series, 2010, , 179-199.	0.5	1
51	Uncontracted Rys Quadrature Implementation of up to G Functions on Graphical Processing Units. Journal of Chemical Theory and Computation, 2010, 6, 696-704.	5.3	95
52	O(³P) + C₂H₄ Potential Energy Surface: Study at the Multireference Level. Journal of Physical Chemistry A, 2009, 113, 12663-12674.	2.5	21
53	A Component Approach to Collaborative Scientific Software Development: Tools and Techniques Utilized by the Quantum Chemistry Science Application Partnership. Scientific Programming, 2008, 16, 287-296.	0.7	2
54	Basis Set Exchange:â€‰ A Community Database for Computational Sciences. Journal of Chemical Information and Modeling, 2007, 47, 1045-1052.	5.4	2,685

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55	A Collaborative Informatics Infrastructure for Multi-Scale Science. Cluster Computing, 2005, 8, 243-253.	5.0	18
56	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
57	6-31G* basis set for atoms K through Zn. Journal of Chemical Physics, 1998, 109, 1223-1229.	3.0	1,766
58	Pinnacle: An approach toward object oriented quantum chemistry. International Journal of Quantum Chemistry, 1995, 56, 485-495.	2.0	14
59	Parallel Implementation of the Electronic Structure Code GAMESS. ACS Symposium Series, 1995, , 16-28.	0.5	5
60	Applications of Parallel GAMESS. ACS Symposium Series, 1995, , 29-46.	0.5	2
61	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	3.3	19,020
62	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. ACS Symposium Series, 0, , 3-53.	0.5	3
63	Rare Earth Elements and Critical Materials: Uses and Availability. ACS Symposium Series, 0, , 63-74.	0.5	1