Lori A Burns

List of Publications by Year
in descending order

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32 papers	5,292 citations	361045 20 h-index	414034 32 g-index
36 all docs	36 docs citations	36 times ranked	5300 citing authors

#	Article	IF	Citations
1	<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.	2.3	961
2	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	6.2	838
3	Density-functional approaches to noncovalent interactions: A comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. Journal of Chemical Physics, 2011, 134, 084107.	1.2	607
4	Levels of symmetry adapted perturbation theory (SAPT). I. Efficiency and performance for interaction energies. Journal of Chemical Physics, 2014, 140, 094106.	1.2	589
5	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
6	Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions. Journal of Chemical Theory and Computation, 2011, 7, 88-96.	2.3	388
7	Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 2197-2203.	2.1	305
8	Basis set convergence of the coupled-cluster correction, $delta _{ext{MP2}}^{ext{CCSD(T)}}$ÎMP2CCSD(T): Best practices for benchmarking non-covalent interactions and the attendant revision of the S22, NBC10, HBC6, and HSG databases. Journal of Chemical Physics, 2011, 135, 194102.	1.2	295
9	Comparing Counterpoise-Corrected, Uncorrected, and Averaged Binding Energies for Benchmarking Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 49-57.	2.3	166
10	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
11	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	1.2	82
12	Appointing silver and bronze standards for noncovalent interactions: A comparison of spin-component-scaled (SCS), explicitly correlated (F12), and specialized wavefunction approaches. Journal of Chemical Physics, 2014, 141, 234111.	1.2	81
13	Buckyplates and Buckybowls: Examining the Effects of Curvature on Ï€â€“Ï€ Interactions. Journal of Physical Chemistry A, 2012, 116, 11920-11926.	1.1	58
14	Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 86-99.	2.3	48
15	The <scp>MolSSI</scp> QCA<scp>rchive</scp> project: An openâ€source platform to compute, organize, and share quantum chemistry data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1491.	6.2	42
16	Color-blind fluorescence detection for four-color DNA sequencing. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5346-5351.	3.3	39
17	Investigation of electronic structure and proton transfer in ground state acetylacetone. Chemical Physics Letters, 2007, 434, 31-37.	1.2	25
18	An exploration of electronic structure and nuclear dynamics in tropolone: II. The Ã1ƒâ€‰B12 (Ï€âˆ—Ï€) excited state. Journal of Chemical Physics, 2009, 130, 144304.	1.2	23

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19	Vibrational specificity of proton-transfer dynamics in ground-state tropolone. Physical Chemistry Chemical Physics, 2010, 12, 8285.	1.3	23
20	An exploration of electronic structure and nuclear dynamics in tropolone. I. The XÌƒA11 ground state. Journal of Chemical Physics, 2006, 124, 204307.	1.2	21
21	Redox-Linked Conformational Control of Proton-Coupled Electron Transfer: Y122 in the Ribonucleotide Reductase Î²2 Subunit. Journal of Physical Chemistry B, 2013, 117, 8457-8468.	1.2	18
22	Python implementation of the restrained electrostatic potential charge model. International Journal of Quantum Chemistry, 2020, 120, e26035.	1.0	17
23	Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory. Journal of Chemical Physics, 2020, 152, 124109.	1.2	15
24	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.	1.2	15
25	CrystaLattE: Automated computation of lattice energies of organic crystals exploiting the many-body expansion to achieve dual-level parallelism. Journal of Chemical Physics, 2019, 151, 144103.	1.2	14
26	Electronic Structure and Proton Transfer in Ground-State Hexafluoroacetylacetone. Journal of Physical Chemistry A, 2010, 114, 6630-6640.	1.1	13
27	An Error and Efficiency Analysis of Approximations to MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 3681-3687.	2.3	12
28	Mode-specific tunneling dynamics in the ground electronic state of tropolone. Journal of Chemical Physics, 2007, 127, 081101.	1.2	11
29	Dissection of Rovibronic Structure by Polarization-Resolved Two-Color Resonant Four-Wave Mixing Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 13184-13198.	1.1	9
30	Counterion and Substrate Effects on Barrier Heights of the Hydrolytic Kinetic Resolution of Terminal Epoxides Catalyzed by Co(III)-salen. Journal of Physical Chemistry A, 2015, 119, 403-409.	1.1	9
31	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 234107.	1.2	3
32	Double proton transfer in the and states of the tropolone â€¢ HF complex. Molecular Physics, 2010, 108, 1171-1190.	0.8	2