Susi Lehtola

List of Publications by Year
in descending order

48 papers	3,136 citations	257429 24 h-index	182417 51 g-index
58 all docs	58 docs citations	58 times ranked	2516 citing authors

#	Article	IF	Citations
1	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
2	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
3	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	Recent developments in libxc â€" A comprehensive library of functionals for density functional theory. SoftwareX, 2018, 7, 1-5.	2.6	367
5	Microscopic structure of water at elevated pressures and temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6301-6306.	7.1	127
6	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. Journal of Chemical Theory and Computation, 2020, 16, 2340-2354.	5.3	85
7	Structure of Liquid Linear Alcohols. Journal of Physical Chemistry B, 2010, 114, 6426-6436.	2.6	82
8	Pipekâ€"Mezey Orbital Localization Using Various Partial Charge Estimates. Journal of Chemical Theory and Computation, 2014, 10, 642-649.	5.3	73
9	ERKALEâ€"A flexible program package for Xâ€ray properties of atoms and molecules. Journal of Computational Chemistry, 2012, 33, 1572-1585.	3.3	70
10	Unitary Optimization of Localized Molecular Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 5365-5372.	5.3	69
11	Variational, Self-Consistent Implementation of the Perdewâ€"Zunger Self-Interaction Correction with Complex Optimal Orbitals. Journal of Chemical Theory and Computation, 2014, 10, 5324-5337.	5.3	69
12	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdewâ€"Zunger Self-Interaction Corrected Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2016, 12, 3195-3207.	5.3	54
13	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.0	46
14	A review on nonâ€relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. International Journal of Quantum Chemistry, 2019, 119, e25968.	2.0	45
15	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	5.3	43
16	Assessment of Initial Guesses for Self-Consistent Field Calculations. Superposition of Atomic Potentials: Simple yet Efficient. Journal of Chemical Theory and Computation, 2019, 15, 1593-1604.	5.3	37
17	An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. Molecules, 2020, 25, 1218.	3.8	37
18	Theory and Applications of Generalized Pipekâ€"Mezey Wannier Functions. Journal of Chemical Theory and Computation, 2017, 13, 460-474.	5.3	32

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19	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. Journal of Chemical Physics, 2015, 142, 094114.	3.0	30
20	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdewâ€“Zunger Self-Interaction Correction to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 4296-4302.	5.3	29
21	Fully numerical Hartreeâ€Fock and density functional calculations. I. Atoms. International Journal of Quantum Chemistry, 2019, 119, e25945.	2.0	26
22	Protonation Dynamics and Hydrogen Bonding in Aqueous Sulfuric Acid. Journal of Physical Chemistry B, 2015, 119, 11732-11739.	2.6	25
23	Cluster decomposition of full configuration interaction wave functions: A tool for chemical interpretation of systems with strong correlation. Journal of Chemical Physics, 2017, 147, 154105.	3.0	25
24	Universal Signature of Hydrogen Bonding in the Oxygen K-Edge Spectrum of Alcohols. Journal of Physical Chemistry B, 2010, 114, 13076-13083.	2.6	24
25	Fully numerical Hartreeâ€Fock and density functional calculations. II. Diatomic molecules. International Journal of Quantum Chemistry, 2019, 119, e25944.	2.0	22
26	Curing basis set overcompleteness with pivoted Cholesky decompositions. Journal of Chemical Physics, 2019, 151, 241102.	3.0	22
27	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. Physical Review A, 2020, 101, .	2.5	22
28	DQC: A Python program package for differentiable quantum chemistry. Journal of Chemical Physics, 2022, 156, 084801.	3.0	20
29	Completeness-optimized basis sets: Application to ground-state electron momentum densities. Journal of Chemical Physics, 2012, 137, 104105.	3.0	19
30	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. Molecular Physics, 2020, 118, .	1.7	19
31	Free and open source software for computational chemistry education. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	19
32	Contraction of completeness-optimized basis sets: Application to ground-state electron momentum densities. Journal of Chemical Physics, 2013, 138, 044109.	3.0	18
33	Automatic algorithms for completenessâ€optimization of <scp>G</scp>aussian basis sets. Journal of Computational Chemistry, 2015, 36, 335-347.	3.3	18
34	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hextuples models. Journal of Chemical Physics, 2016, 145, 134110.	3.0	17
35	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. Molecular Physics, 2018, 116, 547-560.	1.7	17
36	PyFLOSIC: Python-based Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2020, 153, 084104.	3.0	17

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37	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	2.5	17
38	Straightforward and Accurate Automatic Auxiliary Basis Set Generation for Molecular Calculations with Atomic Orbital Basis Sets. Journal of Chemical Theory and Computation, 2021, 17, 6886-6900.	5.3	17
39	Calculation of isotropic Compton profiles with Gaussian basis sets. Physical Chemistry Chemical Physics, 2011, 13, 5630.	2.8	16
40	Polarized Gaussian basis sets from one-electron ions. Journal of Chemical Physics, 2020, 152, 134108.	3.0	15
41	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. Procedia Computer Science, 2015, 51, 1858-1864.	2.0	12
42	Accurate reproduction of strongly repulsive interatomic potentials. Physical Review A, 2020, 101, .	2.5	12
43	Efficient implementation of the superposition of atomic potentials initial guess for electronic structure calculations in Gaussian basis sets. Journal of Chemical Physics, 2020, 152, 144105.	3.0	11
44	Gas-Phase Peroxyl Radical Recombination Reactions: AÂComputational Study of Formation and Decomposition of Tetroxides. Journal of Physical Chemistry A, 2022, 126, 4046-4056.	2.5	9
45	Chemical bonding theories as guides for self-interaction corrected solutions: Multiple local minima and symmetry breaking. Journal of Chemical Physics, 2021, 155, 224109.	3.0	7
46	Sulfur Molecules in Space by X-rays: A Computational Study. ACS Earth and Space Chemistry, 2021, 5, 436-448.	2.7	6
47	Meta-Local Density Functionals: A New Rung on Jacobâ€™s Ladder. Journal of Chemical Theory and Computation, 2021, 17, 943-948.	5.3	4
48	Intra- and intermolecular effects on the Compton profile of the ionic liquid 1,3-dimethylimidazolium chloride. Journal of Chemical Physics, 2014, 141, 244505.	3.0	2