Susi Lehtola

List of Publications by Citations

47 papers	1,518 citations	20 h-index	38 g-index
58 ext. papers	2,190 ext. citations	4.2 avg, IF	5.48 L-index

#	Paper	IF	Citations
47	Recent developments in libxc □A comprehensive library of functionals for density functional theory. *SoftwareX*, **2018**, 7, 1-5	2.7	180
46	Psi4 1.4: Open-source software for high-throughput quantum chemistry. *Journal of Chemical Physics* , **2020**, 152, 184108	3.9	158
45	Recent developments in the PySCF program package. *Journal of Chemical Physics*, **2020**, 153, 024109	3.9	121
44	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
43	Microscopic structure of water at elevated pressures and temperatures. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 6301-6	11.5	108
42	Structure of liquid linear alcohols. *Journal of Physical Chemistry B*, **2010**, 114, 6426-36	3.4	73
41	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. *Journal of Chemical Theory and Computation*, **2014**, 10, 5324-37	6.4	59
40	ERKALE-A flexible program package for X-ray properties of atoms and molecules. *Journal of Computational Chemistry*, **2012**, 33, 1572-85	3.5	58
39	Unitary Optimization of Localized Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2013**, 9, 5365-72	6.4	56
38	Pipek-Mezey Orbital Localization Using Various Partial Charge Estimates. *Journal of Chemical Theory and Computation*, **2014**, 10, 642-9	6.4	49
37	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 2340-2354	6.4	44
36	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdew-Zunger Self-Interaction Corrected Density Functional Theory Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3195-207	6.4	39
35	Stretched or noded orbital densities and self-interaction correction in density functional theory. *Journal of Chemical Physics*, **2019**, 150, 174102	3.9	33
34	Theory and Applications of Generalized Pipek-Mezey Wannier Functions. *Journal of Chemical Theory and Computation*, **2017**, 13, 460-474	6.4	25
33	Universal signature of hydrogen bonding in the oxygen K-edge spectrum of alcohols. *Journal of Physical Chemistry B*, **2010**, 114, 13076-83	3.4	24
32	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdew-Zunger Self-Interaction Correction to Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 4296-302	6.4	23
31	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	6.4	23

30	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. *Journal of Chemical Physics*, **2015**, 142, 094114	3.9	22
29	Protonation Dynamics and Hydrogen Bonding in Aqueous Sulfuric Acid. *Journal of Physical Chemistry B*, **2015**, 119, 11732-9	3.4	22
28	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	3.9	20
27	Benchmarking Magnetizabilities with Recent Density Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 1457-1468	6.4	19
26	Completeness-optimized basis sets: application to ground-state electron momentum densities. *Journal of Chemical Physics*, **2012**, 137, 104105	3.9	18
25	Contraction of completeness-optimized basis sets: application to ground-state electron momentum densities. *Journal of Chemical Physics*, **2013**, 138, 044109	3.9	17
24	An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. *Molecules*, **2020**, 25,	4.8	16
23	Calculation of isotropic Compton profiles with Gaussian basis sets. *Physical Chemistry Chemical Physics*, **2011**, 13, 5630-41	3.6	15
22	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hextuples models. *Journal of Chemical Physics*, **2016**, 145, 134110	3.9	15
21	Fully numerical Hartree-Fock and density functional calculations. II. Diatomic molecules. *International Journal of Quantum Chemistry*, **2019**, 119, e25944	2.1	14
20	Automatic algorithms for completeness-optimization of Gaussian basis sets. *Journal of Computational Chemistry*, **2015**, 36, 335-47	3.5	13
19	Curing basis set overcompleteness with pivoted Cholesky decompositions. *Journal of Chemical Physics*, **2019**, 151, 241102	3.9	13
18	A review on non-relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. *International Journal of Quantum Chemistry*, **2019**, 119, e25968	2.1	12
17	Fully numerical Hartree-Fock and density functional calculations. I. Atoms. *International Journal of Quantum Chemistry*, **2019**, 119, e25945	2.1	12
16	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. *Molecular Physics*, **2020**, 118, e1597989	1.7	10
15	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. *Molecular Physics*, **2018**, 116, 547-560	1.7	10
14	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. *Procedia Computer Science*, **2015**, 51, 1858-1864	1.6	9
13	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. *Physical Review A*, **2020**, 101,	2.6	8

12	PyFLOSIC: Python-based Fermi-Löwdin orbital self-interaction correction. *Journal of Chemical Physics*, **2020**, 153, 084104	3.9	8
11	Spatial Contributions to Nuclear Magnetic Shieldings. *Journal of Physical Chemistry A*, **2021**, 125, 1778-1786	2.8	8
10	Accurate reproduction of strongly repulsive interatomic potentials. *Physical Review A*, **2020**, 101,	2.6	7
9	Polarized Gaussian basis sets from one-electron ions. *Journal of Chemical Physics*, **2020**, 152, 134108	3.9	5
8	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	3.9	5
7	DQC: A Python program package for differentiable quantum chemistry.. *Journal of Chemical Physics*, **2022**, 156, 084801	3.9	5
6	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	6.4	3
5	Free and Open Source Software for Computational Chemistry Education		3
4	Intra- and intermolecular effects on the Compton profile of the ionic liquid 1,3-dimethylimidazolium chloride. *Journal of Chemical Physics*, **2014**, 141, 244505	3.9	2
3	Chemical bonding theories as guides for self-interaction corrected solutions: Multiple local minima and symmetry breaking.. *Journal of Chemical Physics*, **2021**, 155, 224109	3.9	2
2	Sulfur Molecules in Space by X-rays: A Computational Study. *ACS Earth and Space Chemistry*, **2021**, 5, 436-448	3.2	1
1	Meta-Local Density Functionals: A New Rung on Jacob's Ladder. *Journal of Chemical Theory and Computation*, **2021**, 17, 943-948	6.4	0