

Susi Lehtola

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	DQC: A Python program package for differentiable quantum chemistry.. <i>Journal of Chemical Physics</i> , 2022 , 156, 084801	3.9	5
46	Chemical bonding theories as guides for self-interaction corrected solutions: Multiple local minima and symmetry breaking.. <i>Journal of Chemical Physics</i> , 2021 , 155, 224109	3.9	2
45	Straightforward and Accurate Automatic Auxiliary Basis Set Generation for Molecular Calculations with Atomic Orbital Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6886-6900	6.4	3
44	Meta-Local Density Functionals: A New Rung on Jacob's Ladder. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 943-948	6.4	0
43	Sulfur Molecules in Space by X-rays: A Computational Study. <i>ACS Earth and Space Chemistry</i> , 2021 , 5, 436-448	3.2	1
42	Spatial Contributions to Nuclear Magnetic Shieldings. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 1778-1786	2.8	8
41	Benchmarking Magnetizabilities with Recent Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1457-1468	6.4	19
40	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021 , 155, 084801	3.9	115
39	Psi4 1.4: Open-source software for high-throughput quantum chemistry. <i>Journal of Chemical Physics</i> , 2020 , 152, 184108	3.9	158
38	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. <i>Physical Review A</i> , 2020 , 101,	2.6	8
37	An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. <i>Molecules</i> , 2020 , 25,	4.8	16
36	Accurate reproduction of strongly repulsive interatomic potentials. <i>Physical Review A</i> , 2020 , 101,	2.6	7
35	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2340-2354	6.4	44
34	Polarized Gaussian basis sets from one-electron ions. <i>Journal of Chemical Physics</i> , 2020 , 152, 134108	3.9	5
33	Efficient implementation of the superposition of atomic potentials initial guess for electronic structure calculations in Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2020 , 152, 144105	3.9	5
32	Recent developments in the PySCF program package. <i>Journal of Chemical Physics</i> , 2020 , 153, 024109	3.9	121
31	PyFLOSIC: Python-based Fermi-Löwdin orbital self-interaction correction. <i>Journal of Chemical Physics</i> , 2020 , 153, 084104	3.9	8

30	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. <i>Molecular Physics</i> , 2020 , 118, e1597989	1.7	10
29	A review on non-relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25968	2.1	12
28	Stretched or noded orbital densities and self-interaction correction in density functional theory. <i>Journal of Chemical Physics</i> , 2019 , 150, 174102	3.9	33
27	Fully numerical Hartree-Fock and density functional calculations. II. Diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25944	2.1	14
26	Fully numerical Hartree-Fock and density functional calculations. I. Atoms. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25945	2.1	12
25	Curing basis set overcompleteness with pivoted Cholesky decompositions. <i>Journal of Chemical Physics</i> , 2019 , 151, 241102	3.9	13
24	Assessment of Initial Guesses for Self-Consistent Field Calculations. Superposition of Atomic Potentials: Simple yet Efficient. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1593-1604	6.4	23
23	Recent developments in libxc: A comprehensive library of functionals for density functional theory. <i>SoftwareX</i> , 2018 , 7, 1-5	2.7	180
22	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. <i>Molecular Physics</i> , 2018 , 116, 547-560	1.7	10
21	Theory and Applications of Generalized Pipek-Mezey Wannier Functions. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 460-474	6.4	25
20	Cluster decomposition of full configuration interaction wave functions: A tool for chemical interpretation of systems with strong correlation. <i>Journal of Chemical Physics</i> , 2017 , 147, 154105	3.9	20
19	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdew-Zunger Self-Interaction Correction to Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4296-302	6.4	23
18	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hexuples models. <i>Journal of Chemical Physics</i> , 2016 , 145, 134110	3.9	15
17	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdew-Zunger Self-Interaction Corrected Density Functional Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3195-207	6.4	39
16	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. <i>Procedia Computer Science</i> , 2015 , 51, 1858-1864	1.6	9
15	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. <i>Journal of Chemical Physics</i> , 2015 , 142, 094114	3.9	22
14	Automatic algorithms for completeness-optimization of Gaussian basis sets. <i>Journal of Computational Chemistry</i> , 2015 , 36, 335-47	3.5	13
13	Protonation Dynamics and Hydrogen Bonding in Aqueous Sulfuric Acid. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11732-9	3.4	22

12	Pipek-Mezey Orbital Localization Using Various Partial Charge Estimates. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 642-9	6.4	49
11	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5324-37	6.4	59
10	Intra- and intermolecular effects on the Compton profile of the ionic liquid 1,3-dimethylimidazolium chloride. <i>Journal of Chemical Physics</i> , 2014 , 141, 244505	3.9	2
9	Unitary Optimization of Localized Molecular Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5365-72	6.4	56
8	Microscopic structure of water at elevated pressures and temperatures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 6301-6	11.5	108
7	Contraction of completeness-optimized basis sets: application to ground-state electron momentum densities. <i>Journal of Chemical Physics</i> , 2013 , 138, 044109	3.9	17
6	Completeness-optimized basis sets: application to ground-state electron momentum densities. <i>Journal of Chemical Physics</i> , 2012 , 137, 104105	3.9	18
5	ERKALE-A flexible program package for X-ray properties of atoms and molecules. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1572-85	3.5	58
4	Calculation of isotropic Compton profiles with Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 5630-41	3.6	15
3	Universal signature of hydrogen bonding in the oxygen K-edge spectrum of alcohols. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 13076-83	3.4	24
2	Structure of liquid linear alcohols. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 6426-36	3.4	73
1	Free and Open Source Software for Computational Chemistry Education		3