Andrew M Teale

List of Publications by Year
in descending order

65 papers	3,068 citations	201674 27 h-index	161849 54 g-index
67 all docs	67 docs citations	67 times ranked	2554 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Benchmarking density-functional theory calculations of NMR shielding constants and spinâ€“rotation constants using accurate coupled-cluster calculations. Journal of Chemical Physics, 2013, 138, 024111.	3.0	153
3	Orbital energies and negative electron affinities from density functional theory: Insight from the integer discontinuity. Journal of Chemical Physics, 2008, 129, 044110.	3.0	112
4	Accurate calculation and modeling of the adiabatic connection in density functional theory. Journal of Chemical Physics, 2010, 132, 164115.	3.0	86
5	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. Journal of Chemical Physics, 2014, 140, 034101.	3.0	67
6	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2015, 11, 4169-4181.	5.3	66
7	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	3.0	64
8	Exchange representations in Kohnâ€“Sham NMR shielding calculations. Chemical Physics Letters, 2004, 383, 109-114.	2.6	62
9	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. Journal of Chemical Physics, 2009, 131, 144104.	3.0	60
10	Choice of basic variables in current-density-functional theory. Physical Review A, 2012, 86, .	2.5	52
11	Maps of current density using density-functional methods. Journal of Chemical Physics, 2008, 129, 074101.	3.0	50
12	Differentiable but exact formulation of density-functional theory. Journal of Chemical Physics, 2014, 140, 18A518.	3.0	48
13	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	2.6	42
14	Analysis of double-hybrid density functionals along the adiabatic connection. Molecular Physics, 2013, 111, 1275-1294.	1.7	42
15	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. Journal of Physical Chemistry A, 2020, 124, 1321-1333.	2.5	42
16	The intramolecular Î²-fluorineâ‹¯ammonium interaction in 4- and 8-membered rings. Chemical Communications, 2006, , 3190-3192.	4.1	41
17	Exchangeâ€“Correlation Functionals via Local Interpolation along the Adiabatic Connection. Journal of Chemical Theory and Computation, 2016, 12, 2598-2610.	5.3	40
18	Comparing ab initio density-functional and wave function theories: The impact of correlation on the electronic density and the role of the correlation potential. Journal of Chemical Physics, 2011, 135, 114111.	3.0	39

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19	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	3.0	38
20	Fractional Electron Loss in Approximate DFT and Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2015, 11, 5262-5268.	5.3	38
21	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. Journal of Chemical Physics, 2013, 139, 134113.	3.0	37
22	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. Journal of Chemical Physics, 2014, 141, 024113.	3.0	35
23	The importance of current contributions to shielding constants in density-functional theory. Physical Chemistry Chemical Physics, 2015, 17, 18834-18842.	2.8	35
24	Efficient Calculation of Molecular Integrals over London Atomic Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 3636-3649.	5.3	35
25	Modeling the adiabatic connection in H2. Journal of Chemical Physics, 2007, 126, 244104.	3.0	34
26	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. Journal of Chemical Theory and Computation, 2017, 13, 4089-4100.	5.3	32
27	Range-dependent adiabatic connections. Journal of Chemical Physics, 2010, 133, 164112.	3.0	30
28	Optimizing Molecular Geometries in Strong Magnetic Fields. Journal of Chemical Theory and Computation, 2021, 17, 2166-2185.	5.3	29
29	Interpolated energy densities, correlation indicators and lower bounds from approximations to the strong coupling limit of DFT. Physical Chemistry Chemical Physics, 2017, 19, 6169-6183.	2.8	28
30	Effective homogeneity of the exchangeâ€“correlation and non-interacting kinetic energy functionals under density scaling. Journal of Chemical Physics, 2012, 136, 034101.	3.0	25
31	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	1.7	25
32	Modeling Ultrafast Electron Dynamics in Strong Magnetic Fields Using Real-Time Time-Dependent Electronic Structure Methods. Journal of Chemical Theory and Computation, 2021, 17, 2137-2165.	5.3	25
33	Transition metal NMR chemical shifts from optimized effective potentials. Journal of Chemical Physics, 2007, 126, 074101.	3.0	22
34	Adiabatic connection forms in density functional theory: H2 and the He isoelectronic series. Journal of Chemical Physics, 2008, 129, 064105.	3.0	21
35	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. Journal of Chemical Physics, 2011, 135, 194109.	3.0	21
36	Kohnâ€“Sham energy decomposition for molecules in a magnetic field. Molecular Physics, 2019, 117, 97-109.	1.7	21

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37	GW quasiparticle energies of atoms in strong magnetic fields. Journal of Chemical Physics, 2019, 150, 214112.	3.0	21
38	Uniform magnetic fields in density-functional theory. Journal of Chemical Physics, 2018, 148, 024101.	3.0	20
39	Exchange methods in Kohnâ€“Sham theory. Physical Chemistry Chemical Physics, 2005, 7, 2991.	2.8	19
40	Shielding Constants and Chemical Shifts in DFT: Influence of Optimized Effective Potential and Coulomb-Attenuation. Journal of Physical Chemistry A, 2010, 114, 7179-7186.	2.5	18
41	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	3.0	17
42	Self-Consistent Field Methods for Excited States in Strong Magnetic Fields: a Comparison between Energy- and Variance-Based Approaches. Journal of Chemical Theory and Computation, 2021, 17, 5492-5508.	5.3	16
43	Accelerating Kohnâ€Sham response theory using density fitting and the auxiliaryâ€densityâ€matrix method. International Journal of Quantum Chemistry, 2018, 118, e25639.	2.0	15
44	RotationalgTensors Calculated Using Hybrid Exchange-Correlation Functionals with the Optimized Effective Potential Approach. Journal of Chemical Theory and Computation, 2006, 2, 827-834.	5.3	14
45	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	2.5	14
46	Electron localisation function in current-density-functional theory. Molecular Physics, 2016, 114, 1415-1422.	1.7	14
47	New CHARMM force field parameters for dehydrated amino acid residues, the key to lantibiotic molecular dynamics simulations. RSC Advances, 2014, 4, 48621-48631.	3.6	13
48	Ground- and excited-state diatomic bond lengths, vibrational levels, and potential-energy curves from conventional and localized Hartreeâ€“Fock-based density-functional theory. Journal of Chemical Physics, 2005, 122, 034101.	3.0	12
49	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	1.7	12
50	Revisiting the density scaling of the non-interacting kinetic energy. Physical Chemistry Chemical Physics, 2014, 16, 14578-14583.	2.8	11
51	Revealing the exotic structure of molecules in strong magnetic fields. Journal of Chemical Physics, 2022, 156, .	3.0	11
52	Atomic electron affinities and the role of symmetry between electron addition and subtraction in a corrected Koopmans approach. Physical Chemistry Chemical Physics, 2014, 16, 14420-14434.	2.8	9
53	Molecular properties in the Tammâ€“Dancoff approximation: indirect nuclear spinâ€“spin coupling constants. Molecular Physics, 2015, 113, 1937-1951.	1.7	9
54	The coupling constant averaged exchangeâ€“correlation energy density. Molecular Physics, 0, , 1-14.	1.7	9

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55	Topological Analysis of Magnetically Induced Current Densities in Strong Magnetic Fields Using Stagnation Graphs. Chemistry, 2021, 3, 916-934.	2.2	9
56	Robust All-Electron Optimization in Orbital-Free Density-Functional Theory Using the Trust-Region Image Method. Journal of Physical Chemistry A, 2021, 125, 459-475.	2.5	8
57	Alternative Representations of the Correlation Energy in Densityâ€Functional Theory: A Kineticâ€Energy Based Adiabatic Connection. Journal of the Chinese Chemical Society, 2016, 63, 121-128.	1.4	7
58	Excitation energies from GÃ¶rlingâ€“Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	1.7	5
59	Connections between variation principles at the interface of wave-function and density-functional theories. Journal of Chemical Physics, 2017, 147, 134107.	3.0	4
60	Structural and electronic studies of substituted m-terphenyl lithium complexes. Dalton Transactions, 2021, 50, 722-728.	3.3	4
61	High accuracy ab initio studies of electron-densities for the ground state of Be-like atomic systems. Journal of Chemical Physics, 2013, 138, 164306.	3.0	3
62	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
63	Structural and Electronic Studies of Substituted m-Terphenyl Group 12 Complexes. Organometallics, 0, , .	2.3	2
64	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
65	Range-dependent adiabatic connections. , 2012, , .		0