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	Revealing the exotic structure of molecules in strong magnetic fields. Journal of Chemical Physics, 2022, 156, .	3.0	11
2	Optimizing Molecular Geometries in Strong Magnetic Fields. Journal of Chemical Theory and Computation, 2021, 17, 2166-2185.	5.3	29
3	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
4	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
5	Topological Analysis of Magnetically Induced Current Densities in Strong Magnetic Fields Using Stagnation Graphs. Chemistry, 2021, 3, 916-934.	2.2	9
6	Structural and electronic studies of substituted m-terphenyl lithium complexes. Dalton Transactions, 2021, 50, 722-728.	3.3	4
7	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
8	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. Journal of Physical Chemistry A, 2020, 124, 1321-1333.	2.5	42
9	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
10	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
11	Kohnâ€“Sham energy decomposition for molecules in a magnetic field. Molecular Physics, 2019, 117, 97-109.	1.7	21
12	GW quasiparticle energies of atoms in strong magnetic fields. Journal of Chemical Physics, 2019, 150, 214112.	3.0	21
13	Excitation energies from GÃ¶rlingâ€“Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	1.7	5
14	Uniform magnetic fields in density-functional theory. Journal of Chemical Physics, 2018, 148, 024101.	3.0	20
15	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
16	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
17	Connections between variation principles at the interface of wave-function and density-functional theories. Journal of Chemical Physics, 2017, 147, 134107.	3.0	4
18	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. Journal of Chemical Theory and Computation, 2017, 13, 4089-4100.	5.3	32

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19	Efficient Calculation of Molecular Integrals over London Atomic Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 3636-3649.	5.3	35
20	Exchangeâ€“Correlation Functionals via Local Interpolation along the Adiabatic Connection. Journal of Chemical Theory and Computation, 2016, 12, 2598-2610.	5.3	40
21	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
22	Electron localisation function in current-density-functional theory. Molecular Physics, 2016, 114, 1415-1422.	1.7	14
23	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	1.7	12
24	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2015, 11, 4169-4181.	5.3	66
25	The importance of current contributions to shielding constants in density-functional theory. Physical Chemistry Chemical Physics, 2015, 17, 18834-18842.	2.8	35
26	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	2.5	14
27	Molecular properties in the Tammâ€“Dancoff approximation: indirect nuclear spinâ€“spin coupling constants. Molecular Physics, 2015, 113, 1937-1951.	1.7	9
28	Fractional Electron Loss in Approximate DFT and Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2015, 11, 5262-5268.	5.3	38
29	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
30	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. Journal of Chemical Physics, 2014, 140, 034101.	3.0	67
31	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
32	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	1.7	25
33	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	3.0	17
34	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
35	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
36	Revisiting the density scaling of the non-interacting kinetic energy. Physical Chemistry Chemical Physics, 2014, 16, 14578-14583.	2.8	11

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37	Differentiable but exact formulation of density-functional theory. Journal of Chemical Physics, 2014, 140, 18A518.	3.0	48
38	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	3.0	38
39	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
40	Analysis of double-hybrid density functionals along the adiabatic connection. Molecular Physics, 2013, 111, 1275-1294.	1.7	42
41	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
42	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
43	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
44	Choice of basic variables in current-density-functional theory. Physical Review A, 2012, 86, .	2.5	52
45	Range-dependent adiabatic connections. , 2012, , .		0
46	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. Journal of Chemical Physics, 2011, 135, 194109.	3.0	21
47	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
48	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	2.6	42
49	Range-dependent adiabatic connections. Journal of Chemical Physics, 2010, 133, 164112.	3.0	30
50	Accurate calculation and modeling of the adiabatic connection in density functional theory. Journal of Chemical Physics, 2010, 132, 164115.	3.0	86
51	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
52	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
53	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	3.0	64
54	Maps of current density using density-functional methods. Journal of Chemical Physics, 2008, 129, 074101.	3.0	50

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55	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
56	Adiabatic connection forms in density functional theory: H2 and the He isoelectronic series. Journal of Chemical Physics, 2008, 129, 064105.	3.0	21
57	Modeling the adiabatic connection in H2. Journal of Chemical Physics, 2007, 126, 244104.	3.0	34
58	Transition metal NMR chemical shifts from optimized effective potentials. Journal of Chemical Physics, 2007, 126, 074101.	3.0	22
59	The intramolecular Î²-fluorineâ‹¯ammonium interaction in 4- and 8-membered rings. Chemical Communications, 2006, , 3190-3192.	4.1	41
60	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
61	Exchange methods in Kohnâ€“Sham theory. Physical Chemistry Chemical Physics, 2005, 7, 2991.	2.8	19
62	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
63	Exchange representations in Kohnâ€“Sham NMR shielding calculations. Chemical Physics Letters, 2004, 383, 109-114.	2.6	62
64	The coupling constant averaged exchangeâ€“correlation energy density. Molecular Physics, 0, , 1-14.	1.7	9
65	Structural and Electronic Studies of Substituted m-Terphenyl Group 12 Complexes. Organometallics, 0, , .	2.3	2