Andrew M Teale

List of Publications by Citations

62 papers	2,430 citations	23 h-index	48 g-index
67 ext. papers	2,765 ext. citations	3.7 avg, IF	4.8 L-index

#	Paper	IF	Citations
62	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
61	Benchmarking density-functional theory calculations of NMR shielding constants and spin-rotation constants using accurate coupled-cluster calculations. *Journal of Chemical Physics*, **2013**, 138, 024111	3.9	119
60	Orbital energies and negative electron affinities from density functional theory: Insight from the integer discontinuity. *Journal of Chemical Physics*, **2008**, 129, 044110	3.9	104
59	Accurate calculation and modeling of the adiabatic connection in density functional theory. *Journal of Chemical Physics*, **2010**, 132, 164115	3.9	77
58	The calculation of adiabatic-connection curves from full configuration-interaction densities: two-electron systems. *Journal of Chemical Physics*, **2009**, 130, 104111	3.9	59
57	Exchange representations in KohnSham NMR shielding calculations. *Chemical Physics Letters*, **2004**, 383, 109-114	2.5	56
56	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. *Journal of Chemical Physics*, **2009**, 131, 144104	3.9	47
55	Maps of current density using density-functional methods. *Journal of Chemical Physics*, **2008**, 129, 074101	3.9	45
54	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. *Journal of Chemical Physics*, **2014**, 140, 034101	3.9	43
53	Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153	2.5	41
52	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 4169-81	6.4	40
51	Analysis of double-hybrid density functionals along the adiabatic connection. *Molecular Physics*, **2013**, 111, 1275-1294	1.7	37
50	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	3.9	36
49	Communication: Analytic gradients in the random-phase approximation. *Journal of Chemical Physics*, **2013**, 139, 081101	3.9	34
48	Choice of basic variables in current-density-functional theory. *Physical Review A*, **2012**, 86,	2.6	34
47	The intramolecular beta-fluorine...ammonium interaction in 4- and 8-membered rings. *Chemical Communications*, **2006**, 3190-2	5.8	34
46	Fractional Electron Loss in Approximate DFT and Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5262-8	6.4	33

45	Differentiable but exact formulation of density-functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A518	3.9	31
44	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. *Journal of Chemical Physics*, **2013**, 139, 134113	3.9	30
43	Modeling the adiabatic connection in H2. *Journal of Chemical Physics*, **2007**, 126, 244104	3.9	30
42	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. *Journal of Chemical Physics*, **2014**, 141, 024113	3.9	29
41	Range-dependent adiabatic connections. *Journal of Chemical Physics*, **2010**, 133, 164112	3.9	29
40	Exchange-Correlation Functionals via Local Interpolation along the Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2016**, 12, 2598-610	6.4	29
39	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	3.6	23
38	A density difference based analysis of orbital-dependent exchange-correlation functionals. *Molecular Physics*, **2014**, 112, 700-710	1.7	23
37	The importance of current contributions to shielding constants in density-functional theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 18834-42	3.6	22
36	Efficient Calculation of Molecular Integrals over London Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2017**, 13, 3636-3649	6.4	22
35	Effective homogeneity of the exchange-correlation and non-interacting kinetic energy functionals under density scaling. *Journal of Chemical Physics*, **2012**, 136, 034101	3.9	22
34	Transition metal NMR chemical shifts from optimized effective potentials. *Journal of Chemical Physics*, **2007**, 126, 074101	3.9	21
33	Adiabatic connection forms in density functional theory: H2 and the He isoelectronic series. *Journal of Chemical Physics*, **2008**, 129, 064105	3.9	20
32	Exchange methods in Kohn-Sham theory. *Physical Chemistry Chemical Physics*, **2005**, 7, 2991-8	3.6	19
31	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2017**, 13, 4089-4100	6.4	18
30	Dispersion interactions in density-functional theory: an adiabatic-connection analysis. *Journal of Chemical Physics*, **2011**, 135, 194109	3.9	18
29	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. *Journal of Physical Chemistry A*, **2020**, 124, 1321-1333	2.8	18
28	Excitation energies along a range-separated adiabatic connection. *Journal of Chemical Physics*, **2014**, 141, 044123	3.9	17

27	Shielding constants and chemical shifts in DFT: influence of optimized effective potential and Coulomb-attenuation. *Journal of Physical Chemistry A*, **2010**, 114, 7179-86	2.8	16
26	Calculating excitation energies by extrapolation along adiabatic connections. *Physical Review A*, **2015**, 91,	2.6	14
25	Rotational g Tensors Calculated Using Hybrid Exchange-Correlation Functionals with the Optimized Effective Potential Approach. *Journal of Chemical Theory and Computation*, **2006**, 2, 827-34	6.4	14
24	Optimizing Molecular Geometries in Strong Magnetic Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 2166-2185	6.4	14
23	Uniform magnetic fields in density-functional theory. *Journal of Chemical Physics*, **2018**, 148, 024101	3.9	12
22	Kohn–Sham energy decomposition for molecules in a magnetic field. *Molecular Physics*, **2019**, 117, 97-109	1.7	12
21	Ground- and excited-state diatomic bond lengths, vibrational levels, and potential-energy curves from conventional and localized Hartree-Fock-based density-functional theory. *Journal of Chemical Physics*, **2005**, 122, 34101	3.9	12
20	Excited states from range-separated density-functional perturbation theory. *Molecular Physics*, **2015**, 113, 1740-1749	1.7	11
19	GW quasiparticle energies of atoms in strong magnetic fields. *Journal of Chemical Physics*, **2019**, 150, 214112	3.9	10
18	Electron localisation function in current-density-functional theory. *Molecular Physics*, **2016**, 114, 1415-1422	1.7	10
17	Revisiting the density scaling of the non-interacting kinetic energy. *Physical Chemistry Chemical Physics*, **2014**, 16, 14578-83	3.6	10
16	Atomic electron affinities and the role of symmetry between electron addition and subtraction in a corrected Koopmans approach. *Physical Chemistry Chemical Physics*, **2014**, 16, 14420-34	3.6	9
15	New CHARMM force field parameters for dehydrated amino acid residues, the key to lantibiotic molecular dynamics simulations. *RSC Advances*, **2014**, 4, 48621-48631	3.7	9
14	Accelerating Kohn-Sham response theory using density fitting and the auxiliary-density-matrix method. *International Journal of Quantum Chemistry*, **2018**, 118, e25639	2.1	8
13	Molecular properties in the Tamm–Dancoff approximation: indirect nuclear spin–spin coupling constants. *Molecular Physics*, **2015**, 113, 1937-1951	1.7	7
12	The coupling constant averaged exchange–correlation energy density. *Molecular Physics*, **2015**, 1-14	1.7	7
11	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	6.4	7
10	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	6.4	6

9	Excitation energies from G□ling□levy perturbation theory along the range-separated adiabatic connection. *Molecular Physics*, **2018**, 116, 1443-1451	1.7	4
8	Alternative Representations of the Correlation Energy in Density-Functional Theory: A Kinetic-Energy Based Adiabatic Connection. *Journal of the Chinese Chemical Society*, **2016**, 63, 121-128	1.5	4
7	Topological Analysis of Magnetically Induced Current Densities in Strong Magnetic Fields Using Stagnation Graphs. *Chemistry*, **2021**, 3, 916-934	2.1	4
6	Connections between variation principles at the interface of wave-function and density-functional theories. *Journal of Chemical Physics*, **2017**, 147, 134107	3.9	3
5	High accuracy ab initio studies of electron-densities for the ground state of Be-like atomic systems. *Journal of Chemical Physics*, **2013**, 138, 164306	3.9	2
4	New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508	3.6	2
3	New density-functional approximations and beyond: general discussion. *Faraday Discussions*, **2020**, 224, 166-200	3.6	1
2	Structural and electronic studies of substituted m-terphenyl lithium complexes. *Dalton Transactions* , **2021**, 50, 722-728	4.3	1
1	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	2.8	0