# Andrew M Teale

## List of Publications by Year in Descending Order



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| 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 | 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 |
| 61 | Optimizing Molecular Geometries in Strong Magnetic Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 2166-2185 | 6.4 | 14 |
| 60 | 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 |
| 59 | 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 |
| 58 | Topological Analysis of Magnetically Induced Current Densities in Strong Magnetic Fields Using Stagnation Graphs. *Chemistry*, **2021**, 3, 916-934 | 2.1 | 4 |
| 57 | Structural and electronic studies of substituted m-terphenyl lithium complexes. *Dalton Transactions* , **2021**, 50, 722-728 | 4.3 | 1 |
| 56 | Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. *Journal of Physical Chemistry A*, **2020**, 124, 1321-1333 | 2.8 | 18 |
| 55 | New density-functional approximations and beyond: general discussion. *Faraday Discussions*, **2020**, 224, 166-200 | 3.6 | 1 |
| 54 | New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508 | 3.6 | 2 |
| 53 | GW quasiparticle energies of atoms in strong magnetic fields. *Journal of Chemical Physics*, **2019**, 150, 214112 | 3.9 | 10 |
| 52 | Kohn–Sham energy decomposition for molecules in a magnetic field. *Molecular Physics*, **2019**, 117, 97-109 | 1.7 | 12 |
| 51 | Excitation energies from Görling–Levy perturbation theory along the range-separated adiabatic connection. *Molecular Physics*, **2018**, 116, 1443-1451 | 1.7 | 4 |
| 50 | Uniform magnetic fields in density-functional theory. *Journal of Chemical Physics*, **2018**, 148, 024101 | 3.9 | 12 |
| 49 | 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 |
| 48 | 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 |
| 47 | Connections between variation principles at the interface of wave-function and density-functional theories. *Journal of Chemical Physics*, **2017**, 147, 134107 | 3.9 | 3 |
| 46 | Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2017**, 13, 4089-4100 | 6.4 | 18 |

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| 45 | Efficient Calculation of Molecular Integrals over London Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2017**, 13, 3636-3649 | 6.4 | 22 |
| 44 | 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 |
| 43 | Electron localisation function in current-density-functional theory. *Molecular Physics*, **2016**, 114, 1415-1422 | 1.7 | 10 |
| 42 | Exchange-Correlation Functionals via Local Interpolation along the Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2016**, 12, 2598-610 | 6.4 | 29 |
| 41 | Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 4169-81 | 6.4 | 40 |
| 40 | The importance of current contributions to shielding constants in density-functional theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 18834-42 | 3.6 | 22 |
| 39 | Calculating excitation energies by extrapolation along adiabatic connections. *Physical Review A*, **2015**, 91, | 2.6 | 14 |
| 38 | Molecular properties in the Tamm–Dancoff approximation: indirect nuclear spin–spin coupling constants. *Molecular Physics*, **2015**, 113, 1937-1951 | 1.7 | 7 |
| 37 | Fractional Electron Loss in Approximate DFT and Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5262-8 | 6.4 | 33 |
| 36 | The coupling constant averaged exchange–correlation energy density. *Molecular Physics*, **2015**, 1-14 | 1.7 | 7 |
| 35 | Excited states from range-separated density-functional perturbation theory. *Molecular Physics*, **2015**, 113, 1740-1749 | 1.7 | 11 |
| 34 | The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284 | 7.9 | 956 |
| 33 | A density difference based analysis of orbital-dependent exchange-correlation functionals. *Molecular Physics*, **2014**, 112, 700-710 | 1.7 | 23 |
| 32 | Excitation energies along a range-separated adiabatic connection. *Journal of Chemical Physics*, **2014** , 141, 044123 | 3.9 | 17 |
| 31 | 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 |
| 30 | 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 |
| 29 | Revisiting the density scaling of the non-interacting kinetic energy. *Physical Chemistry Chemical Physics*, **2014**, 16, 14578-83 | 3.6 | 10 |
| 28 | Differentiable but exact formulation of density-functional theory. *Journal of Chemical Physics*, **2014** , 140, 18A518 | 3.9 | 31 |

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| 27 | 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 |
| 26 | Non-perturbative calculation of molecular magnetic properties within current-density functional theory. *Journal of Chemical Physics*, **2014**, 140, 034101 | 3.9 | 43 |
| 25 | Communication: Analytic gradients in the random-phase approximation. *Journal of Chemical Physics* , **2013**, 139, 081101 | 3.9 | 34 |
| 24 | 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 |
| 23 | Analysis of double-hybrid density functionals along the adiabatic connection. *Molecular Physics*, **2013**, 111, 1275-1294 | 1.7 | 37 |
| 22 | 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 |
| 21 | 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 |
| 20 | 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 |
| 19 | Choice of basic variables in current-density-functional theory. *Physical Review A*, **2012**, 86, | 2.6 | 34 |
| 18 | Dispersion interactions in density-functional theory: an adiabatic-connection analysis. *Journal of Chemical Physics*, **2011**, 135, 194109 | 3.9 | 18 |
| 17 | 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 |
| 16 | Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153 | 2.5 | 41 |
| 15 | Range-dependent adiabatic connections. *Journal of Chemical Physics*, **2010**, 133, 164112 | 3.9 | 29 |
| 14 | Accurate calculation and modeling of the adiabatic connection in density functional theory. *Journal of Chemical Physics*, **2010**, 132, 164115 | 3.9 | 77 |
| 13 | 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 |
| 12 | 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 |
| 11 | The calculation of adiabatic-connection curves from full configuration-interaction densities: two-electron systems. *Journal of Chemical Physics*, **2009**, 130, 104111 | 3.9 | 59 |
| 10 | Maps of current density using density-functional methods. *Journal of Chemical Physics*, **2008**, 129, 074101 | 3.9 | 45 |

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| 9 | 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 |
| 8 | Adiabatic connection forms in density functional theory: H2 and the He isoelectronic series. *Journal of Chemical Physics*, **2008**, 129, 064105 | 3.9 | 20 |
| 7 | Modeling the adiabatic connection in H2. *Journal of Chemical Physics*, **2007**, 126, 244104 | 3.9 | 30 |
| 6 | Transition metal NMR chemical shifts from optimized effective potentials. *Journal of Chemical Physics*, **2007**, 126, 074101 | 3.9 | 21 |
| 5 | The intramolecular beta-fluorine...ammonium interaction in 4- and 8-membered rings. *Chemical Communications*, **2006**, 3190-2 | 5.8 | 34 |
| 4 | 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 |
| 3 | Exchange methods in Kohn-Sham theory. *Physical Chemistry Chemical Physics*, **2005**, 7, 2991-8 | 3.6 | 19 |
| 2 | 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 |
| 1 | Exchange representations in KohnSham NMR shielding calculations. *Chemical Physics Letters*, **2004**, 383, 109-114 | 2.5 | 56 |