Anthony D Dutoi

List of Publications by Year
in descending order

19	6,011	686830 13	794141 19
papers	citations	h-index	g-index

19	19	19	7042
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Scaled opposite-spin second order MÃ¸llerâ€“Plesset correlation energy: An economical electronic structure method. Journal of Chemical Physics, 2004, 121, 9793-9802.	1.2	492
4	Self-interaction error of local density functionals for alkaliâ€“halide dissociation. Chemical Physics Letters, 2006, 422, 230-233.	1.2	98
5	Accurate local approximations to the triples correlation energy: formulation, implementation and tests of 5th-order scaling models. Molecular Physics, 2005, 103, 425-437.	0.8	53
6	Tracing molecular electronic excitation dynamics in real time and space. Journal of Chemical Physics, 2010, 132, 144302.	1.2	36
7	Ultrafast charge separation driven by differential particle and hole mobilities. Journal of Chemical Physics, 2011, 134, 024303.	1.2	23
8	Visualising many-body electron dynamics using one-body densities and orbitals. Molecular Physics, 2014, 112, 1-11.	0.8	22
9	A Study of the Effect of Attenuation Curvature on Molecular Correlation Energies by Introducing an Explicit Cutoff Radius into Two-Electron Integrals. Journal of Physical Chemistry A, 2008, 112, 2110-2119.	1.1	19
10	An Excited Electron Avoiding a Positive Charge. Journal of Physical Chemistry Letters, 2011, 2, 2300-2303.	2.1	19
11	Time-resolved pump-probe spectroscopy to follow valence electronic motion in molecules: Theory. Physical Review A, 2013, 88, .	1.0	18
12	Time-resolved pump-probe spectroscopy to follow valence electronic motion in molecules: Application. Physical Review A, 2014, 90, .	1.0	16
13	An Orbital-Based Definition of Radical and Multiradical Character. Journal of Physical Chemistry A, 2004, 108, 10270-10279.	1.1	13
14	Title is missing!. Journal of Chemical Crystallography, 1998, 28, 893-898.	0.5	11
15	Simulation of X-ray transient absorption for following vibrations in coherently ionized F2 molecules. Chemical Physics, 2017, 482, 249-264.	0.9	10
16	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. Chemical Physics Letters, 2009, 478, 283-286.	1.2	9
17	Excitonically renormalised coupled-cluster theory. Molecular Physics, 2019, 117, 446-461.	0.8	5
18	<scp>A2Cloudâ€RF</scp>: A random forest based statistical framework to guide resource selection for <scp>highâ€performance</scp> scientific computing on the cloud. Concurrency Computation Practice and Experience, 2020, 32, e5942.	1.4	5

#	Article	IF	Citations
19	Systematically improvable excitonic Hamiltonians for electronic structure theory. Molecular Physics, 2019, 117, 431-445.	0.8	4