Roger D Amos

List of Publications by Year
in descending order

84 papers	7,184 citations	53794 45 h-index	54911 84 g-index
85 all docs	85 docs citations	85 times ranked	4232 citing authors

#	Article	IF	Citations
1	Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868.	1.7	511
2	Geometric derivatives of excitation energies using SCF and DFT. Chemical Physics Letters, 1999, 308, 249-255.	2.6	357
3	Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals. Chemical Physics Letters, 2000, 317, 159-164.	2.6	330
4	Density Functional Theory for Charge Transfer:Â The Nature of the N-Bands of Porphyrins and Chlorophylls Revealed through CAM-B3LYP, CASPT2, and SAC-CI Calculations. Journal of Physical Chemistry B, 2006, 110, 15624-15632.	2.6	315
5	Calculation of polarizability derivatives using analytic gradient methods. Chemical Physics Letters, 1986, 124, 376-381.	2.6	271
6	Restricted MÃ¸llerâ€"Plesset theory for open-shell molecules. Chemical Physics Letters, 1991, 186, 130-136.	2.6	265
7	The application of CAM-B3LYP to the charge-transfer band problem of the zincbacteriochlorinâ€"bacteriochlorin complex. Chemical Physics Letters, 2006, 420, 106-109.	2.6	256
8	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. Journal of Chemical Physics, 1986, 85, 963-968.	3.0	245
9	Study of methane, acetylene, ethene, and benzene using Kohn-Sham theory. The Journal of Physical Chemistry, 1993, 97, 4392-4396.	2.9	244
10	The harmonic frequencies of benzene. Chemical Physics Letters, 1992, 197, 506-515.	2.6	233
11	The elimination of singularities in derivative calculations. Chemical Physics Letters, 1985, 120, 151-158.	2.6	219
12	On the necessity offbasis functions for bending frequencies. Journal of Chemical Physics, 1988, 88, 3187-3195.	3.0	174
13	Electric and magnetic properties of CO, HF, HCl, and CH3F. Chemical Physics Letters, 1982, 87, 23-26.	2.6	172
14	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. Journal of Chemical Physics, 1992, 97, 4233-4254.	3.0	150
15	Open-shell Mâ^...llerâ€"Plesset perturbation theory. Chemical Physics Letters, 1991, 185, 256-264.	2.6	138
16	Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. Journal of Chemical Physics, 1990, 93, 8828-8839.	3.0	132
17	Kohnâ€"Sham bond lengths and frequencies calculated with accurate quadrature and large basis sets. Chemical Physics Letters, 1992, 199, 551-556.	2.6	128
18	Molecular polarisabilities - a comparison of density functional theory with standard ab initio methods. Chemical Physics Letters, 1995, 235, 1-4.	2.6	125

#	Article	IF	Citations
19	The determination of hyperpolarisabilities using density functional theory. Chemical Physics Letters, 1993, 210, 261-268.	2.6	123
20	SCF and CI calculations of the one-electron properties, polarizabilities and polarizability derivatives of the nitrogen molecule. Molecular Physics, 1980, 39, 1-14.	1.7	105
21	A study of O3, S3, CH2, and Be2 using Kohnâ€“Sham theory with accurate quadrature and large basis sets. Journal of Chemical Physics, 1993, 98, 7145-7151.	3.0	104
22	Nuclear shielding constants by density functional theory with gauge including atomic orbitals. Journal of Chemical Physics, 2000, 113, 2983-2989.	3.0	104
23	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. Journal of Chemical Physics, 1990, 93, 4965-4981.	3.0	101
24	Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868.	1.7	100
25	Analytic Second Derivatives of the Potential Energy Surface. Israel Journal of Chemistry, 1993, 33, 331-344.	2.3	93
26	Spin contamination in single-determinant wavefunctions. Chemical Physics Letters, 1991, 183, 423-431.	2.6	91
27	Molecular Property Derivatives. Advances in Chemical Physics, 2007, , 99-153.	0.3	85
28	Correlated ab initio harmonic frequencies and infrared intensities for furan, pyrrole, and thiophene. The Journal of Physical Chemistry, 1988, 92, 1739-1742.	2.9	82
29	Studies of the Ground and Excited-State Surfaces of the Retinal Chromophore using CAM-B3LYP. Journal of Physical Chemistry B, 2010, 114, 5547-5555.	2.6	79
30	Study of excited states of furan and pyrrole by time-dependent density functional theory. Chemical Physics Letters, 2002, 355, 8-18.	2.6	75
31	Structures, harmonic frequencies and infrared intensities of the dimers of H2O and H2S. Chemical Physics, 1986, 104, 145-151.	1.9	71
32	Toward coupled-cluster accuracy in the prediction of nuclear shielding constants: a simple and efficient DFT approach. Chemical Physics Letters, 1999, 312, 475-484.	2.6	69
33	Kohn-Sham calculations on open-shell diatomic molecules. Molecular Physics, 1993, 80, 1121-1134.	1.7	67
34	Multipole moments and polarizabilities of hydrogen fluoride. A comparison of confguration interaction and perturbation theory methods. Chemical Physics Letters, 1982, 88, 89-94.	2.6	63
35	Gradient theory applied to the Brueckner doubles method. Journal of Chemical Physics, 1991, 95, 6723-6733.	3.0	63
36	Vibrational contributions to static polarizabilities and hyperpolarizabilities. Journal of Chemical Physics, 1994, 100, 4467-4476.	3.0	61

#	Article	IF	Citations
37	Density functional predictions for magnetizabilities and nuclear shielding constants. Molecular Physics, 1999, 97, 757-768.	1.7	58
38	Ab initio ro-vibrational levels of H3+ beyond the Born-Oppenheimer approximation. Chemical Physics Letters, 1995, 232, 295-300.	2.6	57
39	The accurate calculation of molecular properties by ab initio methods. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1247.	1.1	56
40	Higher analytic derivatives. II. The fourth derivative of selfâ€consistentâ€field energy. Journal of Chemical Physics, 1991, 95, 7409-7417.	3.0	55
41	Theory and applications of spin-restricted open-shell MÃ¸ller-Plesset theory. Molecular Physics, 1993, 79, 777-793.	1.7	55
42	Raman intensities using time dependent density functional theory. Physical Chemistry Chemical Physics, 2000, 2, 2123-2129.	2.8	55
43	Comparison of the Brueckner and coupledâ€cluster approaches to electron correlation. Journal of Chemical Physics, 1992, 96, 8931-8937.	3.0	50
44	The calculation of frequency-dependent polarizabilities using current density functional theory. Chemical Physics Letters, 1997, 278, 278-284.	2.6	50
45	A configuration-interaction study of the polarizability derivatives of carbon monoxide. Chemical Physics Letters, 1980, 70, 613-617.	2.6	48
46	The diagonal born-oppenheimer correction for He2+ and F+H2. Chemical Physics Letters, 1996, 251, 52-58.	2.6	48
47	Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: a comparison of standard methods. Chemical Physics Letters, 1998, 291, 71-77.	2.6	45
48	SCF and CI calculations of the one-electron properties of carbon monoxide as a function of internuclear distance. Chemical Physics Letters, 1979, 68, 536-539.	2.6	44
49	Higher analytic derivatives. I. A new implementation for the third derivative of theSCF energy. International Journal of Quantum Chemistry, 1991, 40, 179-199.	2.0	43
50	Structure and vibrational frequencies of diazomethylene (CNN) and diazasilene (SiNN) using nonlocal density functional theory. The Journal of Physical Chemistry, 1993, 97, 1868-1871.	2.9	40
51	Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: an evaluation of DFT functionals. Chemical Physics Letters, 2000, 328, 446-452.	2.6	38
52	Geometries, harmonic frequencies and infrared and Raman intensities for H2O, NH3 and CH4. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1595.	1.1	37
53	Accurate prediction of the properties of materials using the <scp>CAMâ€B3LYP</scp> density functional. Journal of Computational Chemistry, 2021, 42, 1486-1497.	3.3	35
54	Corrections to molecular one-electron properties using mÃ¸ller-plesset perturbation theory. Chemical Physics Letters, 1980, 73, 602-606.	2.6	34

#	Article	IF	Citations
55	Structures and vibrational frequencies of FOOF and FONO using density functional theory. Chemical Physics Letters, 1993, 202, 489-494.	2.6	33
56	Implementation of analytic derivative methods in quantum chemistry. Computer Physics Reports, 1989, 10, 147-187.	2.2	31
57	Higher analytic derivatives. Molecular Physics, 1992, 75, 271-291.	1.7	31
58	Gradient theory applied to restricted (open-shell) MÃ¸llerâ€”Plesset theory. Chemical Physics Letters, 1992, 199, 229-236.	2.6	30
59	Density functional predictions for metal and ligand nuclear shielding constants in diamagnetic closed-shell first-row transition-metal complexes. Physical Chemistry Chemical Physics, 2000, 2, 187-194.	2.8	30
60	Large basis set calculations using Brueckner theory. Journal of Chemical Physics, 1994, 100, 1375-1379.	3.0	28
61	Structure and properties of disilyne. Journal of Chemical Physics, 1993, 98, 7107-7112.	3.0	27
62	Dipole moments in excited state DFT calculations. Chemical Physics Letters, 2002, 364, 612-615.	2.6	27
63	Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes. Molecular Physics, 1992, 77, 381-396.	1.7	26
64	Stationary points on the potential energy surface of (C2H2)3. Chemical Physics Letters, 1989, 161, 166-174.	2.6	23
65	Some investigations of the MP2-R12 method. Theoretica Chimica Acta, 1991, 79, 361-372.	0.8	21
66	The analytic gradient of the perturbative triplet excitations correction to the Brueckner doubles method. Chemical Physics Letters, 1991, 184, 195-202.	2.6	19
67	Comparing long-range corrected functionals in the cisâ€“trans isomerisation of the retinal chromophore. Molecular Physics, 2012, 110, 2329-2336.	1.7	18
68	A theoretical study of hyperpolarizability effects in the measurement of molecular quadrupole moments. Chemical Physics Letters, 1982, 85, 123-125.	2.6	17
69	Ab initio studies of acetylene tetramer and pentamer. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1931.	1.7	17
70	Does fulminic acid have a bent equilibrium structure?. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 755-762.	0.6	16
71	Microsolvation within the Systematic Molecular Fragmentation by Annihilation Approach. Journal of Physical Chemistry A, 2017, 121, 334-341.	2.5	16
72	Electron densities from the Brueckner Doubles method. Theoretica Chimica Acta, 1993, 86, 25-39.	0.8	13

#	Article	IF	Citations
73	Dynamic CCSD polarisabilities of CHF3 and CHCl3. Chemical Physics Letters, 1996, 253, 373-376.	2.6	13
74	Time-dependent density functional theory applied to Raman scattering from methane. Chemical Physics Letters, 1997, 279, 17-21.	2.6	13
75	Ab Initio NMR Chemical Shift Calculations Using Fragment Molecular Orbitals and Locally Dense Basis Sets. Journal of Physical Chemistry A, 2016, 120, 8907-8915.	2.5	13
76	Multipole moments and polarizabulities of cyclopropane. Chemical Physics Letters, 1981, 84, 104-106.	2.6	12
77	Theoretical investigation of the isomerisation of merocyanine. Molecular Physics, 2013, 111, 1574-1579.	1.7	12
78	Analytic second derivatives with model potentials at SCF and MP2 levels. Chemical Physics Letters, 1989, 163, 151-156.	2.6	11
79	Implementation of analytic derivative density functional theory codes on scalar and parallel architectures. AIP Conference Proceedings, 1995, , .	0.4	7
80	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials. Chemical Science, 2022, 13, 1492-1503.	7.4	7
81	Ab initio investigation of the structures and energies of spiropyran and merocyanine isomers. Molecular Physics, 2015, 113, 1674-1681.	1.7	4
82	Spin-coupled wavefunctions. Molecular Physics, 1975, 29, 1125-1135.	1.7	3
83	Spin-coupled wavefunctions. Molecular Physics, 1975, 29, 1117-1124.	1.7	3
84	The use of symmetry in direct Mï¿½ller-Plesset second-order calculations. Theoretica Chimica Acta, 1993, 86, 279-284.	0.8	1