

Roger D Amos

List of Publications by Year in descending order

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84
papers

7,184
citations

53794

45
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54911

84
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85
all docs

85
docs citations

85
times ranked

4232
citing authors

#	ARTICLE	IF	CITATIONS
1	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials. <i>Chemical Science</i> , 2022, 13, 1492-1503.	7.4	7
2	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. <i>Journal of Computational Chemistry</i> , 2021, 42, 1486-1497.	3.3	35
3	Microsolvation within the Systematic Molecular Fragmentation by Annihilation Approach. <i>Journal of Physical Chemistry A</i> , 2017, 121, 334-341.	2.5	16
4	Ab Initio NMR Chemical Shift Calculations Using Fragment Molecular Orbitals and Locally Dense Basis Sets. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8907-8915.	2.5	13
5	Ab initio investigation of the structures and energies of spiropyran and merocyanine isomers. <i>Molecular Physics</i> , 2015, 113, 1674-1681.	1.7	4
6	Theoretical investigation of the isomerisation of merocyanine. <i>Molecular Physics</i> , 2013, 111, 1574-1579.	1.7	12
7	Comparing long-range corrected functionals in the cis \rightarrow trans isomerisation of the retinal chromophore. <i>Molecular Physics</i> , 2012, 110, 2329-2336.	1.7	18
8	Studies of the Ground and Excited-State Surfaces of the Retinal Chromophore using CAM-B3LYP. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5547-5555.	2.6	79
9	Molecular Property Derivatives. <i>Advances in Chemical Physics</i> , 2007, , 99-153.	0.3	85
10	Density Functional Theory for Charge Transfer: The Nature of the N-Bands of Porphyrins and Chlorophylls Revealed through CAM-B3LYP, CASPT2, and SAC-CI Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15624-15632.	2.6	315
11	The application of CAM-B3LYP to the charge-transfer band problem of the zincbacteriochlorin \rightarrow bacteriochlorin complex. <i>Chemical Physics Letters</i> , 2006, 420, 106-109.	2.6	256
12	Study of excited states of furan and pyrrole by time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2002, 355, 8-18.	2.6	75
13	Dipole moments in excited state DFT calculations. <i>Chemical Physics Letters</i> , 2002, 364, 612-615.	2.6	27
14	Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: an evaluation of DFT functionals. <i>Chemical Physics Letters</i> , 2000, 328, 446-452.	2.6	38
15	Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals. <i>Chemical Physics Letters</i> , 2000, 317, 159-164.	2.6	330
16	Nuclear shielding constants by density functional theory with gauge including atomic orbitals. <i>Journal of Chemical Physics</i> , 2000, 113, 2983-2989.	3.0	104
17	Raman intensities using time dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2123-2129.	2.8	55
18	Density functional predictions for metal and ligand nuclear shielding constants in diamagnetic closed-shell first-row transition-metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 187-194.	2.8	30

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19	Geometric derivatives of excitation energies using SCF and DFT. Chemical Physics Letters, 1999, 308, 249-255.	2.6	357
20	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
21	Density functional predictions for magnetizabilities and nuclear shielding constants. Molecular Physics, 1999, 97, 757-768.	1.7	58
22	Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868.	1.7	511
23	Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868.	1.7	100
24	Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: a comparison of standard methods. Chemical Physics Letters, 1998, 291, 71-77.	2.6	45
25	The calculation of frequency-dependent polarizabilities using current density functional theory. Chemical Physics Letters, 1997, 278, 278-284.	2.6	50
26	Time-dependent density functional theory applied to Raman scattering from methane. Chemical Physics Letters, 1997, 279, 17-21.	2.6	13
27	The diagonal born-oppenheimer correction for He ₂ ⁺ and F+H ₂ . Chemical Physics Letters, 1996, 251, 52-58.	2.6	48
28	Dynamic CCSD polarisabilities of CHF ₃ and CHCl ₃ . Chemical Physics Letters, 1996, 253, 373-376.	2.6	13
29	Implementation of analytic derivative density functional theory codes on scalar and parallel architectures. AIP Conference Proceedings, 1995, , .	0.4	7
30	Ab initio ro-vibrational levels of H ₃ ⁺ beyond the Born-Oppenheimer approximation. Chemical Physics Letters, 1995, 232, 295-300.	2.6	57
31	Molecular polarisabilities - a comparison of density functional theory with standard ab initio methods. Chemical Physics Letters, 1995, 235, 1-4.	2.6	125
32	Vibrational contributions to static polarizabilities and hyperpolarizabilities. Journal of Chemical Physics, 1994, 100, 4467-4476.	3.0	61
33	Large basis set calculations using Brueckner theory. Journal of Chemical Physics, 1994, 100, 1375-1379.	3.0	28
34	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
35	The determination of hyperpolarisabilities using density functional theory. Chemical Physics Letters, 1993, 210, 261-268.	2.6	123
36	Structures and vibrational frequencies of FOOF and FONO using density functional theory. Chemical Physics Letters, 1993, 202, 489-494.	2.6	33

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37	Electron densities from the Brueckner Doubles method. <i>Theoretica Chimica Acta</i> , 1993, 86, 25-39.	0.8	13
38	The use of symmetry in direct Møller-Plesset second-order calculations. <i>Theoretica Chimica Acta</i> , 1993, 86, 279-284.	0.8	1
39	Study of methane, acetylene, ethene, and benzene using Kohn-Sham theory. <i>The Journal of Physical Chemistry</i> , 1993, 97, 4392-4396.	2.9	244
40	Analytic Second Derivatives of the Potential Energy Surface. <i>Israel Journal of Chemistry</i> , 1993, 33, 331-344.	2.3	93
41	Structure and vibrational frequencies of diazomethylene (CNN) and diazasilene (SiNN) using nonlocal density functional theory. <i>The Journal of Physical Chemistry</i> , 1993, 97, 1868-1871.	2.9	40
42	Kohn-Sham calculations on open-shell diatomic molecules. <i>Molecular Physics</i> , 1993, 80, 1121-1134.	1.7	67
43	A study of O ₃ , S ₃ , CH ₂ , and Be ₂ using Kohn-Sham theory with accurate quadrature and large basis sets. <i>Journal of Chemical Physics</i> , 1993, 98, 7145-7151.	3.0	104
44	Theory and applications of spin-restricted open-shell Møller-Plesset theory. <i>Molecular Physics</i> , 1993, 79, 777-793.	1.7	55
45	Structure and properties of disilyne. <i>Journal of Chemical Physics</i> , 1993, 98, 7107-7112.	3.0	27
46	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. <i>Journal of Chemical Physics</i> , 1992, 97, 4233-4254.	3.0	150
47	Comparison of the Brueckner and coupled-cluster approaches to electron correlation. <i>Journal of Chemical Physics</i> , 1992, 96, 8931-8937.	3.0	50
48	Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes. <i>Molecular Physics</i> , 1992, 77, 381-396.	1.7	26
49	Higher analytic derivatives. <i>Molecular Physics</i> , 1992, 75, 271-291.	1.7	31
50	Gradient theory applied to restricted (open-shell) Møller-Plesset theory. <i>Chemical Physics Letters</i> , 1992, 199, 229-236.	2.6	30
51	Kohn-Sham bond lengths and frequencies calculated with accurate quadrature and large basis sets. <i>Chemical Physics Letters</i> , 1992, 199, 551-556.	2.6	128
52	The harmonic frequencies of benzene. <i>Chemical Physics Letters</i> , 1992, 197, 506-515.	2.6	233
53	Higher analytic derivatives. II. The fourth derivative of self-consistent-field energy. <i>Journal of Chemical Physics</i> , 1991, 95, 7409-7417.	3.0	55
54	Gradient theory applied to the Brueckner doubles method. <i>Journal of Chemical Physics</i> , 1991, 95, 6723-6733.	3.0	63

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55	Open-shell Møller-Plesset perturbation theory. <i>Chemical Physics Letters</i> , 1991, 185, 256-264.	2.6	138
56	Restricted Møller-Plesset theory for open-shell molecules. <i>Chemical Physics Letters</i> , 1991, 186, 130-136.	2.6	265
57	The analytic gradient of the perturbative triplet excitations correction to the Brueckner doubles method. <i>Chemical Physics Letters</i> , 1991, 184, 195-202.	2.6	19
58	Spin contamination in single-determinant wavefunctions. <i>Chemical Physics Letters</i> , 1991, 183, 423-431.	2.6	91
59	Higher analytic derivatives. I. A new implementation for the third derivative of the SCF energy. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 179-199.	2.0	43
60	Some investigations of the MP2-R12 method. <i>Theoretica Chimica Acta</i> , 1991, 79, 361-372.	0.8	21
61	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH ₃ . <i>Journal of Chemical Physics</i> , 1990, 93, 4965-4981.	3.0	101
62	Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. <i>Journal of Chemical Physics</i> , 1990, 93, 8828-8839.	3.0	132
63	Ab initio studies of acetylene tetramer and pentamer. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1990, 86, 1931.	1.7	17
64	Analytic second derivatives with model potentials at SCF and MP2 levels. <i>Chemical Physics Letters</i> , 1989, 163, 151-156.	2.6	11
65	Stationary points on the potential energy surface of (C ₂ H ₂) ₃ . <i>Chemical Physics Letters</i> , 1989, 161, 166-174.	2.6	23
66	Implementation of analytic derivative methods in quantum chemistry. <i>Computer Physics Reports</i> , 1989, 10, 147-187.	2.2	31
67	The accurate calculation of molecular properties by ab initio methods. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1988, 84, 1247.	1.1	56
68	Correlated ab initio harmonic frequencies and infrared intensities for furan, pyrrole, and thiophene. <i>The Journal of Physical Chemistry</i> , 1988, 92, 1739-1742.	2.9	82
69	On the necessity of basis functions for bending frequencies. <i>Journal of Chemical Physics</i> , 1988, 88, 3187-3195.	3.0	174
70	Geometries, harmonic frequencies and infrared and Raman intensities for H ₂ O, NH ₃ and CH ₄ . <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1987, 83, 1595.	1.1	37
71	Calculation of polarizability derivatives using analytic gradient methods. <i>Chemical Physics Letters</i> , 1986, 124, 376-381.	2.6	271
72	Structures, harmonic frequencies and infrared intensities of the dimers of H ₂ O and H ₂ S. <i>Chemical Physics</i> , 1986, 104, 145-151.	1.9	71

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73	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. <i>Journal of Chemical Physics</i> , 1986, 85, 963-968.	3.0	245
74	The elimination of singularities in derivative calculations. <i>Chemical Physics Letters</i> , 1985, 120, 151-158.	2.6	219
75	Multipole moments and polarizabilities of hydrogen fluoride. A comparison of configuration interaction and perturbation theory methods. <i>Chemical Physics Letters</i> , 1982, 88, 89-94.	2.6	63
76	A theoretical study of hyperpolarizability effects in the measurement of molecular quadrupole moments. <i>Chemical Physics Letters</i> , 1982, 85, 123-125.	2.6	17
77	Electric and magnetic properties of CO, HF, HCl, and CH3F. <i>Chemical Physics Letters</i> , 1982, 87, 23-26.	2.6	172
78	Multipole moments and polarizabilities of cyclopropane. <i>Chemical Physics Letters</i> , 1981, 84, 104-106.	2.6	12
79	A configuration-interaction study of the polarizability derivatives of carbon monoxide. <i>Chemical Physics Letters</i> , 1980, 70, 613-617.	2.6	48
80	Corrections to molecular one-electron properties using Møller-plesset perturbation theory. <i>Chemical Physics Letters</i> , 1980, 73, 602-606.	2.6	34
81	SCF and CI calculations of the one-electron properties, polarizabilities and polarizability derivatives of the nitrogen molecule. <i>Molecular Physics</i> , 1980, 39, 1-14.	1.7	105
82	SCF and CI calculations of the one-electron properties of carbon monoxide as a function of internuclear distance. <i>Chemical Physics Letters</i> , 1979, 68, 536-539.	2.6	44
83	Spin-coupled wavefunctions. <i>Molecular Physics</i> , 1975, 29, 1125-1135.	1.7	3
84	Spin-coupled wavefunctions. <i>Molecular Physics</i> , 1975, 29, 1117-1124.	1.7	3