# Roger D Amos

List of Publications by Year
in descending order

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| 84 | 7,184 | 53660 | 54797 |
|---|---|---|---|
| papers | citations | 45 h-index | 84 g-index |

| 85 | 85 | 85 | 4232 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials. Chemical Science, 2022, 13, 1492-1503. | 3.7 | 7 |
| 2 | Accurate prediction of the properties of materials using the <scp>CAMâ€B3LYP</scp> density functional. Journal of Computational Chemistry, 2021, 42, 1486-1497. | 1.5 | 35 |
| 3 | Microsolvation within the Systematic Molecular Fragmentation by Annihilation Approach. Journal of Physical Chemistry A, 2017, 121, 334-341. | 1.1 | 16 |
| 4 | Ab Initio NMR Chemical Shift Calculations Using Fragment Molecular Orbitals and Locally Dense Basis Sets. Journal of Physical Chemistry A, 2016, 120, 8907-8915. | 1.1 | 13 |
| 5 | Ab initio investigation of the structures and energies of spiropyran and merocyanine isomers. Molecular Physics, 2015, 113, 1674-1681. | 0.8 | 4 |
| 6 | Theoretical investigation of the isomerisation of merocyanine. Molecular Physics, 2013, 111, 1574-1579. | 0.8 | 12 |
| 7 | Comparing long-range corrected functionals in the cisâ€“trans isomerisation of the retinal chromophore. Molecular Physics, 2012, 110, 2329-2336. | 0.8 | 18 |
| 8 | Studies of the Ground and Excited-State Surfaces of the Retinal Chromophore using CAM-B3LYP. Journal of Physical Chemistry B, 2010, 114, 5547-5555. | 1.2 | 79 |
| 9 | Molecular Property Derivatives. Advances in Chemical Physics, 2007, , 99-153. | 0.3 | 85 |
| 10 | 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. | 1.2 | 315 |
| 11 | The application of CAM-B3LYP to the charge-transfer band problem of the zincbacteriochlorinâ€“bacteriochlorin complex. Chemical Physics Letters, 2006, 420, 106-109. | 1.2 | 256 |
| 12 | Study of excited states of furan and pyrrole by time-dependent density functional theory. Chemical Physics Letters, 2002, 355, 8-18. | 1.2 | 75 |
| 13 | Dipole moments in excited state DFT calculations. Chemical Physics Letters, 2002, 364, 612-615. | 1.2 | 27 |
| 14 | Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: an evaluation of DFT functionals. Chemical Physics Letters, 2000, 328, 446-452. | 1.2 | 38 |
| 15 | Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals. Chemical Physics Letters, 2000, 317, 159-164. | 1.2 | 330 |
| 16 | Nuclear shielding constants by density functional theory with gauge including atomic orbitals. Journal of Chemical Physics, 2000, 113, 2983-2989. | 1.2 | 104 |
| 17 | Raman intensities using time dependent density functional theory. Physical Chemistry Chemical Physics, 2000, 2, 2123-2129. | 1.3 | 55 |
| 18 | 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. | 1.3 | 30 |

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|---|---|---|---|
| 19 | Geometric derivatives of excitation energies using SCF and DFT. Chemical Physics Letters, 1999, 308, 249-255. | 1.2 | 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. | 1.2 | 69 |
| 21 | Density functional predictions for magnetizabilities and nuclear shielding constants. Molecular Physics, 1999, 97, 757-768. | 0.8 | 58 |
| 22 | Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868. | 0.8 | 511 |
| 23 | Does density functional theory contribute to the understanding of excited states of unsaturated organic compounds?. Molecular Physics, 1999, 97, 859-868. | 0.8 | 100 |
| 24 | Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: a comparison of standard methods. Chemical Physics Letters, 1998, 291, 71-77. | 1.2 | 45 |
| 25 | The calculation of frequency-dependent polarizabilities using current density functional theory. Chemical Physics Letters, 1997, 278, 278-284. | 1.2 | 50 |
| 26 | Time-dependent density functional theory applied to Raman scattering from methane. Chemical Physics Letters, 1997, 279, 17-21. | 1.2 | 13 |
| 27 | The diagonal born-oppenheimer correction for He2+ and F+H2. Chemical Physics Letters, 1996, 251, 52-58. | 1.2 | 48 |
| 28 | Dynamic CCSD polarisabilities of CHF3 and CHCl3. Chemical Physics Letters, 1996, 253, 373-376. | 1.2 | 13 |
| 29 | Implementation of analytic derivative density functional theory codes on scalar and parallel architectures. AIP Conference Proceedings, 1995, , . | 0.3 | 7 |
| 30 | Ab initio ro-vibrational levels of H3+ beyond the Born-Oppenheimer approximation. Chemical Physics Letters, 1995, 232, 295-300. | 1.2 | 57 |
| 31 | Molecular polarisabilities - a comparison of density functional theory with standard ab initio methods. Chemical Physics Letters, 1995, 235, 1-4. | 1.2 | 125 |
| 32 | Vibrational contributions to static polarizabilities and hyperpolarizabilities. Journal of Chemical Physics, 1994, 100, 4467-4476. | 1.2 | 61 |
| 33 | Large basis set calculations using Brueckner theory. Journal of Chemical Physics, 1994, 100, 1375-1379. | 1.2 | 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. | 1.2 | 123 |
| 36 | Structures and vibrational frequencies of FOOF and FONO using density functional theory. Chemical Physics Letters, 1993, 202, 489-494. | 1.2 | 33 |

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|---|---|---|---|
| 37 | Electron densities from the Brueckner Doubles method. Theoretica Chimica Acta, 1993, 86, 25-39. | 0.9 | 13 |
| 38 | The use of symmetry in direct Mï¿½ller-Plesset second-order calculations. Theoretica Chimica Acta, 1993, 86, 279-284. | 0.9 | 1 |
| 39 | Study of methane, acetylene, ethene, and benzene using Kohn-Sham theory. The Journal of Physical Chemistry, 1993, 97, 4392-4396. | 2.9 | 244 |
| 40 | Analytic Second Derivatives of the Potential Energy Surface. Israel Journal of Chemistry, 1993, 33, 331-344. | 1.0 | 93 |
| 41 | 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 |
| 42 | Kohn-Sham calculations on open-shell diatomic molecules. Molecular Physics, 1993, 80, 1121-1134. | 0.8 | 67 |
| 43 | 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. | 1.2 | 104 |
| 44 | Theory and applications of spin-restricted open-shell MÃ¸ller-Plesset theory. Molecular Physics, 1993, 79, 777-793. | 0.8 | 55 |
| 45 | Structure and properties of disilyne. Journal of Chemical Physics, 1993, 98, 7107-7112. | 1.2 | 27 |
| 46 | Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. Journal of Chemical Physics, 1992, 97, 4233-4254. | 1.2 | 150 |
| 47 | Comparison of the Brueckner and coupledâ€cluster approaches to electron correlation. Journal of Chemical Physics, 1992, 96, 8931-8937. | 1.2 | 50 |
| 48 | Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes. Molecular Physics, 1992, 77, 381-396. | 0.8 | 26 |
| 49 | Higher analytic derivatives. Molecular Physics, 1992, 75, 271-291. | 0.8 | 31 |
| 50 | Gradient theory applied to restricted (open-shell) MÃ¸llerâ€”Plesset theory. Chemical Physics Letters, 1992, 199, 229-236. | 1.2 | 30 |
| 51 | Kohnâ€”Sham bond lengths and frequencies calculated with accurate quadrature and large basis sets. Chemical Physics Letters, 1992, 199, 551-556. | 1.2 | 128 |
| 52 | The harmonic frequencies of benzene. Chemical Physics Letters, 1992, 197, 506-515. | 1.2 | 233 |
| 53 | Higher analytic derivatives. II. The fourth derivative of selfâ€consistentâ€field energy. Journal of Chemical Physics, 1991, 95, 7409-7417. | 1.2 | 55 |
| 54 | Gradient theory applied to the Brueckner doubles method. Journal of Chemical Physics, 1991, 95, 6723-6733. | 1.2 | 63 |

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|---|---|---|---|
| 55 | Open-shell Mâ^...llerâ€"Plesset perturbation theory. Chemical Physics Letters, 1991, 185, 256-264. | 1.2 | 138 |
| 56 | Restricted MÃ¸llerâ€"Plesset theory for open-shell molecules. Chemical Physics Letters, 1991, 186, 130-136. | 1.2 | 265 |
| 57 | The analytic gradient of the perturbative triplet excitations correction to the Brueckner doubles method. Chemical Physics Letters, 1991, 184, 195-202. | 1.2 | 19 |
| 58 | Spin contamination in single-determinant wavefunctions. Chemical Physics Letters, 1991, 183, 423-431. | 1.2 | 91 |
| 59 | Higher analytic derivatives. I. A new implementation for the third derivative of theSCF energy. International Journal of Quantum Chemistry, 1991, 40, 179-199. | 1.0 | 43 |
| 60 | Some investigations of the MP2-R12 method. Theoretica Chimica Acta, 1991, 79, 361-372. | 0.9 | 21 |
| 61 | The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. Journal of Chemical Physics, 1990, 93, 4965-4981. | 1.2 | 101 |
| 62 | Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. Journal of Chemical Physics, 1990, 93, 8828-8839. | 1.2 | 132 |
| 63 | Ab initio studies of acetylene tetramer and pentamer. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1931. | 1.7 | 17 |
| 64 | Analytic second derivatives with model potentials at SCF and MP2 levels. Chemical Physics Letters, 1989, 163, 151-156. | 1.2 | 11 |
| 65 | Stationary points on the potential energy surface of (C2H2)3. Chemical Physics Letters, 1989, 161, 166-174. | 1.2 | 23 |
| 66 | Implementation of analytic derivative methods in quantum chemistry. Computer Physics Reports, 1989, 10, 147-187. | 2.3 | 31 |
| 67 | The accurate calculation of molecular properties by ab initio methods. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1247. | 1.1 | 56 |
| 68 | 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 |
| 69 | On the necessity offbasis functions for bending frequencies. Journal of Chemical Physics, 1988, 88, 3187-3195. | 1.2 | 174 |
| 70 | 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 |
| 71 | Calculation of polarizability derivatives using analytic gradient methods. Chemical Physics Letters, 1986, 124, 376-381. | 1.2 | 271 |
| 72 | Structures, harmonic frequencies and infrared intensities of the dimers of H2O and H2S. Chemical Physics, 1986, 104, 145-151. | 0.9 | 71 |

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|---|---|---|---|
| 73 | 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. | 1.2 | 245 |
| 74 | The elimination of singularities in derivative calculations. Chemical Physics Letters, 1985, 120, 151-158. | 1.2 | 219 |
| 75 | Multipole moments and polarizabilities of hydrogen fluoride. A comparison of confguration interaction and perturbation theory methods. Chemical Physics Letters, 1982, 88, 89-94. | 1.2 | 63 |
| 76 | A theoretical study of hyperpolarizability effects in the measurement of molecular quadrupole moments. Chemical Physics Letters, 1982, 85, 123-125. | 1.2 | 17 |
| 77 | Electric and magnetic properties of CO, HF, HCl, and CH3F. Chemical Physics Letters, 1982, 87, 23-26. | 1.2 | 172 |
| 78 | Multipole moments and polarizabulities of cyclopropane. Chemical Physics Letters, 1981, 84, 104-106. | 1.2 | 12 |
| 79 | A configuration-interaction study of the polarizability derivatives of carbon monoxide. Chemical Physics Letters, 1980, 70, 613-617. | 1.2 | 48 |
| 80 | Corrections to molecular one-electron properties using mÃ¸ller-plesset perturbation theory. Chemical Physics Letters, 1980, 73, 602-606. | 1.2 | 34 |
| 81 | SCF and CI calculations of the one-electron properties, polarizabilities and polarizability derivatives of the nitrogen molecule. Molecular Physics, 1980, 39, 1-14. | 0.8 | 105 |
| 82 | 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. | 1.2 | 44 |
| 83 | Spin-coupled wavefunctions. Molecular Physics, 1975, 29, 1125-1135. | 0.8 | 3 |
| 84 | Spin-coupled wavefunctions. Molecular Physics, 1975, 29, 1117-1124. | 0.8 | 3 |