George Fitzgerald

List of Publications by Year
in descending order

25 papers	3,691 citations	361045 20 h-index	580395 25 g-index
25 all docs	25 docs citations	25 times ranked	3316 citing authors

#	Article	IF	Citations
1	Use of approximate integrals in ab initio theory. An application in MP2 energy calculations. Chemical Physics Letters, 1993, 208, 359-363.	1.2	1,116
2	A generalized synchronous transit method for transition state location. Computational Materials Science, 2003, 28, 250-258.	1.4	1,050
3	Molecular gradients and hessians implemented in density functional theory. Journal of Chemical Physics, 1993, 98, 1398-1421.	1.2	200
4	Geometry optimization of solids using delocalized internal coordinates. Chemical Physics Letters, 2001, 335, 321-326.	1.2	167
5	Chemical bonding in water clusters. Journal of Chemical Physics, 1995, 102, 1266-1269.	1.2	131
6	Is fifth-order MBPT enough?. Chemical Physics Letters, 1985, 113, 151-158.	1.2	106
7	Analytic energy gradients for general coupledâ€cluster methods and fourthâ€order manyâ€body perturbation theory. Journal of Chemical Physics, 1986, 85, 5143-5150.	1.2	95
8	Analytic energy second derivatives for general MCSCF wave functions. Journal of Chemical Physics, 1984, 80, 2660-2668.	1.2	87
9	Density functional pseudopotential studies of molecular geometries, vibrations, and binding energies. Journal of Chemical Physics, 1993, 98, 8710-8717.	1.2	86
10	Theory and application of MBPT(3) gradients: The density approach. Chemical Physics Letters, 1987, 141, 61-70.	1.2	82
11	Structures of the water hexamer using density functional methods. Journal of Chemical Physics, 1994, 101, 4472-4473.	1.2	71
12	Analytic energy second derivatives for general correlated wavefunctions, including a solution of the first-order coupled-perturbed configuration-interaction equations. Chemical Physics Letters, 1983, 102, 17-19.	1.2	63
13	Analytical gradient evaluation in coupled-cluster theory. Chemical Physics Letters, 1985, 117, 433-436.	1.2	57
14	Zeolite-Catalyzed Hydrocarbon Formation from Methanol: Density Functional Simulations. International Journal of Molecular Sciences, 2002, 3, 423-434.	1.8	51
15	Analytic force constants for postâ€Hartreeâ€“Fock wave functions: The simplest case. Journal of Chemical Physics, 1983, 78, 1607-1608.	1.2	49
16	Thirdâ€order MBPT gradients. Journal of Chemical Physics, 1985, 82, 4379-4380.	1.2	49
17	DFT study of methanol conversion to hydrocarbons in a zeolite catalyst. International Journal of Quantum Chemistry, 2003, 91, 467-473.	1.0	46
18	Electron correlation studies of SiC2. Journal of Chemical Physics, 1986, 85, 1701-1703.	1.2	42

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19	Ionization of Bases in Water:Â Structure and Stability of the NH4+Â·Â·Â·OH-Ionic Forms in Ammoniaâ^'Water Clusters. The Journal of Physical Chemistry, 1996, 100, 7398-7404.	2.9	41
20	Analytic energy derivative methods for excited singlet states of the same symmetry as the electronic ground state. Journal of Chemical Physics, 1985, 83, 1162-1167.	1.2	21
21	The cyclic, twoâ€hydrogen bond form of the HO2 dimer. Journal of Chemical Physics, 1984, 81, 362-367.	1.2	20
22	Nonlocal density functional calculations: Comparison of two implementation schemes. Journal of Chemical Physics, 1993, 98, 2971-2974.	1.2	20
23	An investigation of hydrogen transfer in water clusters. Journal of Chemical Physics, 1996, 104, 5555-5557.	1.2	20
24	Structures, Energetics and Vibrational Frequencies of Cyclopropyne. Israel Journal of Chemistry, 1983, 23, 93-96.	1.0	14
25	A Spectroscopic and Computational Investigation of the Vanadomolybdate Local Structure in the Lyonsite Phase Mg_{2.5}VMoO₈. Inorganic Chemistry, 2007, 46, 6556-6564.	1.9	7