Jacek Kobus

List of Publications by Year
in descending order

37 papers	847 citations	471509 17 h-index	477307 29 g-index
37 all docs	37 docs citations	37 times ranked	482 citing authors

#	Article	IF	Citations
1	Numerical Hartreeâ€“Fock and Many-Body Calculations for Diatomic Molecules. Advances in Quantum Chemistry, 2018, 76, 103-116.	0.8	2
2	Interatomic Coulombic Decay: The Mechanism for Rapid Deexcitation of Hollow Atoms. Physical Review Letters, 2017, 119, 103401.	7.8	69
3	Numerical Methods for Solving the Hartree-Fock Equations of Diatomic Molecules II. Communications in Computational Physics, 2016, 19, 632-647.	1.7	3
4	Hartree-Fock limit values of multipole moments, polarizabilities, and hyperpolarizabilities for atoms and diatomic molecules. Physical Review A, 2015, 91, .	2.5	12
5	A numerical solution of the pair equation of a model twoâ€electron diatomic system. International Journal of Quantum Chemistry, 2015, 115, 868-874.	2.0	3
6	A finite difference Hartreeâ€“Fock program for atoms and diatomic molecules. Computer Physics Communications, 2013, 184, 799-811.	7.5	30
7	Overview of finite difference Hartree-Fock method algorithm, implementation and application. AIP Conference Proceedings, 2012, , .	0.4	3
8	Distributed Gaussian basis sets: a comparison with finite difference Hartreeâ€“Fock calculations for potential energy curves of H₂, LiH and BH. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 205102.	1.5	9
9	Comparison of the polarizabilities and hyperpolarizabilities obtained from finite basis set and finite difference Hartreeâ€“Fock calculations for diatomic molecules: III. The ground states of N2, CO and BF. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 877-896.	1.5	17
10	Bond centred functions in relativistic and non-relativistic calculations for diatomics. Chemical Physics, 2006, 321, 277-284.	1.9	6
11	Comparison of the polarizabilities and hyperpolarizabilities obtained from finite basis set and finite difference Hartreeâ€“Fock calculations for diatomic molecules: II. Refinement of basis sets and grids for hyperpolarizability calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 571-585.	1.5	9
12	Relativistic and correlation effects on spectroscopic constants of the hydrogen astatide molecule. Chemical Physics Letters, 2003, 369, 441-448.	2.6	9
13	Three-photon resonances due to autoionizing states in calcium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1801-1817.	1.5	18
14	A comparison of finite basis set and finite difference Hartreeâ€”Fock calculations for the open-shell (X2Î£+) molecules BaF and YbF. Molecular Physics, 2002, 100, 499-508.	1.7	3
15	A relativistic crystal field for S-state f electron ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 1513-1522.	1.5	15
16	Comparison of the polarizabilities and hyperpolarizabilities obtained from finite basis set and finite difference Hartree-Fock calculations for diatomic molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 5127-5143.	1.5	24
17	A comparison of finite difference and finite basis set Hartree-Fock calculations for the N2molecule with finite nuclei. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2045-2056.	1.5	7
18	Comparison of the electric moments obtained from finite basis set and finite-difference Hartree-Fock calculations for diatomic molecules. Physical Review A, 2000, 62, .	2.5	35

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19	Three-photon ionization of Ca. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2259-2278.	1.5	15
20	A comparison of finite basis set and finite difference Hartree-Fock calculations for the InF and TlF molecules. Molecular Physics, 1998, 93, 713-725.	1.7	10
21	Diatomic Molecules: Exact Solutions of HF Equations. Advances in Quantum Chemistry, 1997, , 1-14.	0.8	33
22	Visualization of deficiencies in approximate molecular wave functions: the orbital amplitude difference function for the matrix Hartree-Fock description of the ground state of the boron fluoride molecule. Molecular Physics, 1997, 92, 1015-1028.	1.7	4
23	A numerical Hartree-Fock program for diatomic molecules. Computer Physics Communications, 1996, 98, 346-358.	7.5	123
24	A universal basis set for high precision electronic structure studies. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 4555-4557.	1.5	40
25	A comparison of finite basis set and finite difference Hartree-Fock calculations for the BF, AlF and GaF molecules. Molecular Physics, 1995, 86, 1315-1330.	1.7	39
26	A comparison of finite difference and finite basis set Hartree-Fock calculations for the ground state potential energy curve of CO. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 5139-5147.	1.5	46
27	Vectorizable algorithm for the (multicolour) successive overrelaxation method. Computer Physics Communications, 1994, 78, 247-255.	7.5	33
28	A comparison of finite basis set and finite difference methods for the ground state of the CS molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 2867-2875.	1.5	44
29	Finite-difference versus finite-element methods. Chemical Physics Letters, 1993, 202, 7-12.	2.6	78
30	Comment on "A comparison of relativistic and quasirelativistic line strengths" by A. K. Mohanty and D. H. Sampson. Physica Scripta, 1988, 38, 554-556.	2.5	3
31	Quasirelativistic calculations of the elastic scattering of slow electrons from Xe atoms. Physica Scripta, 1987, 36, 436-440.	2.5	3
32	Matrix elements of rqfor quasirelativistic and Dirac hydrogenic wavefunctions. Journal of Physics A, 1987, 20, 3347-3352.	1.6	24
33	Numerical comparison between DHF and RHF methods. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 4949-4961.	1.6	6
34	The dirac second-order equation and an improved quasirelativistic theory of atoms. International Journal of Quantum Chemistry, 1986, 30, 809-819.	2.0	23
35	Quasirelativistic methods. International Journal of Quantum Chemistry, 1985, 28, 741-756.	2.0	32
36	An effective quasirelativistic hamiltonian. Chemical Physics, 1981, 55, 361-369.	1.9	17

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37	Two-dimensional, finite-difference method of solving the Dirac equation for diatomic molecules revisited. Molecular Physics, 0, , .	1.7	0