Kenneth G Dyall

List of Publications by Year
in descending order

27 papers	3,535 citations	257450 24 h-index	526287 27 g-index

27 all docs	27 docs citations	27 times ranked	1389 citing authors

#	Article	IF	Citations
1	An exact separation of the spinâ€free and spinâ€dependent terms of the Diracâ€“Coulombâ€“Breit Hamiltonian. Journal of Chemical Physics, 1994, 100, 2118-2127.	3.0	501
2	Relativistic Quadruple-Zeta and Revised Triple-Zeta and Double-Zeta Basis Sets for the 4p, 5p, and 6p Elements. Theoretical Chemistry Accounts, 2006, 115, 441-447.	1.4	357
3	Formulation and implementation of a relativistic unrestricted coupledâ€cluster method including noniterative connected triples. Journal of Chemical Physics, 1996, 105, 8769-8776.	3.0	254
4	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the 5d elements Hf?Hg. Theoretical Chemistry Accounts, 2004, 112, 403-409.	1.4	229
5	Relativistic and nonrelativistic finite nucleus optimized triple-zeta basis sets for the 4 p , 5 p and 6 p elements. Theoretical Chemistry Accounts, 2002, 108, 335-340.	1.4	200
6	The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104.	3.0	191
7	Interfacing relativistic and nonrelativistic methods. IV. One- and two-electron scalar approximations. Journal of Chemical Physics, 2001, 115, 9136-9143.	3.0	175
8	Relativistic Double-Zeta, Triple-Zeta, and Quadruple-Zeta Basis Sets for the 4s, 5s, 6s, and 7s Elements. Journal of Physical Chemistry A, 2009, 113, 12638-12644.	2.5	153
9	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the 4d elements Yâ€“Cd. Theoretical Chemistry Accounts, 2007, 117, 483-489.	1.4	150
10	Revised relativistic basis sets for the 5d elements Hfâ€“Hg. Theoretical Chemistry Accounts, 2010, 125, 97-100.	1.4	136
11	Relativistic fourâ€component multiconfigurational selfâ€consistentâ€field theory for molecules: Formalism. Journal of Chemical Physics, 1996, 104, 4083-4097.	3.0	121
12	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the actinides Acâ€“Lr. Theoretical Chemistry Accounts, 2007, 117, 491-500.	1.4	119
13	Relativistic and nonrelativistic finite nucleus optimized double zeta basis sets for the 4. Theoretical Chemistry Accounts, 1998, 99, 366.	1.4	119
14	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the lanthanides Laâ€“Lu. Theoretical Chemistry Accounts, 2010, 127, 369-381.	1.4	107
15	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the light elements Hâ€“Ar. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	94
16	Kinetic balance and variational bounds failure in the solution of the Dirac equation in a finite Gaussian basis set. Chemical Physics Letters, 1990, 174, 25-32.	2.6	92
17	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	2.5	86
18	Core correlating basis functions for elements 31â€“118. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	84

#	Article	IF	Citations
19	Optimization of Gaussian basis sets for Diracâ€“Hartreeâ€“Fock calculations. Theoretica Chimica Acta, 1996, 94, 39.	0.8	75
20	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the 6d elements Rfâ€“Cn. Theoretical Chemistry Accounts, 2011, 129, 603-613.	1.4	74
21	Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the 7p elements, with atomic and molecular applications. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	63
22	Relativistic and nonrelativistic finite nucleus optimized double zeta basis sets for the 4 p , 5 p and 6 p elements (Theor Chem Acc (1998) 99:366-371): addendum. Theoretical Chemistry Accounts, 2002, 108, 365-365.	1.4	57
23	Electron correlation within the relativistic no-pair approximation. Journal of Chemical Physics, 2016, 145, 074104.	3.0	41
24	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	2.6	28
25	Communication: Spectral representation of the Lamb shift for atomic and molecular calculations. Journal of Chemical Physics, 2013, 139, 021103.	3.0	14
26	Semi-segmented contraction of generally contracted basis sets by property minimization. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
27	Electronic spectra of ytterbium fluoride from relativistic electronic structure calculations. Physical Chemistry Chemical Physics, 2021, 23, 22330-22343.	2.8	6