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	Electronic spectra of ytterbium fluoride from relativistic electronic structure calculations. Physical Chemistry Chemical Physics, 2021, 23, 22330-22343.	2.8	6
2	The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104.	3.0	191
3	Electron correlation within the relativistic no-pair approximation. Journal of Chemical Physics, 2016, 145, 074104.	3.0	41
4	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
5	Semi-segmented contraction of generally contracted basis sets by property minimization. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
6	Communication: Spectral representation of the Lamb shift for atomic and molecular calculations. Journal of Chemical Physics, 2013, 139, 021103.	3.0	14
7	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
8	Core correlating basis functions for elements 31â€“118. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	84
9	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
10	Revised relativistic basis sets for the 5d elements Hfâ€“Hg. Theoretical Chemistry Accounts, 2010, 125, 97-100.	1.4	136
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

#	Article	IF	Citations
19	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	2.6	28
20	Interfacing relativistic and nonrelativistic methods. IV. One- and two-electron scalar approximations. Journal of Chemical Physics, 2001, 115, 9136-9143.	3.0	175
21	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	2.5	86
22	Relativistic and nonrelativistic finite nucleus optimized double zeta basis sets for the 4. Theoretical Chemistry Accounts, 1998, 99, 366.	1.4	119
23	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
24	Relativistic fourâ€component multiconfigurational selfâ€consistentâ€field theory for molecules: Formalism. Journal of Chemical Physics, 1996, 104, 4083-4097.	3.0	121
25	Optimization of Gaussian basis sets for Diracâ€“Hartreeâ€“Fock calculations. Theoretica Chimica Acta, 1996, 94, 39.	0.8	75
26	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
27	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