Klaus Ruedenberg

List of Publications by Year
in descending order

118 papers	9,969 citations	46984 47 h-index	34964 98 g-index
127 all docs	127 docs citations	127 times ranked	4000 citing authors

#	Article	IF	Citations
1	Atoms and interatomic bonding synergism inherent in molecular electronic wave functions. Journal of Chemical Physics, 2022, 157, .	1.2	9
2	Multiple Bonding in Rhodium Monoboride. Quasi-atomic Analyses of the Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2021, 125, 4836-4846.	1.1	16
3	Why is Si₂H₂ Not Linear? An Intrinsic Quasi-Atomic Bonding Analysis. Journal of the American Chemical Society, 2020, 142, 13729-13742.	6.6	19
4	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
5	Quasi-Atomic Bond Analyses in the Sixth Period: I. Relativistic Accurate Atomic Minimal Basis Sets for the Elements Cesium to Radon. Journal of Physical Chemistry A, 2019, 123, 5242-5248.	1.1	11
6	Quasi-Atomic Bond Analyses in the Sixth Period: II. Bond Analyses of Cerium Oxides. Journal of Physical Chemistry A, 2019, 123, 5249-5256.	1.1	18
7	Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. Journal of Physical Chemistry A, 2018, 122, 3442-3454.	1.1	18
8	The Virial Theorem and Covalent Bonding. Journal of Physical Chemistry A, 2018, 122, 7880-7893.	1.1	43
9	Correlation Energy Extrapolation by Many-Body Expansion. Journal of Physical Chemistry A, 2017, 121, 836-844.	1.1	23
10	Intrinsic Resolution of Molecular Electronic Wave Functions and Energies in Terms of Quasi-atoms and Their Interactions. Journal of Physical Chemistry A, 2017, 121, 1086-1105.	1.1	44
11	Relativistic ab Initio Accurate Atomic Minimal Basis Sets: Quantitative LUMOs and Oriented Quasi-Atomic Orbitals for the Elements Liâ€“Xe. Journal of Physical Chemistry A, 2017, 121, 3588-3597.	1.1	18
12	Dispersion Interactions in QM/EFP. Journal of Physical Chemistry A, 2017, 121, 9495-9507.	1.1	23
13	Identification and Characterization of Molecular Bonding Structures by ab initio Quasi-Atomic Orbital Analyses. Journal of Physical Chemistry A, 2017, 121, 8884-8898.	1.1	23
14	The transition from the open minimum to the ring minimum on the ground state and on the lowest excited state of like symmetry in ozone: A configuration interaction study. Journal of Chemical Physics, 2016, 144, 104304.	1.2	13
15	Seniority number description of potential energy surfaces: Symmetric dissociation of water, N2, C2, and Be2. Journal of Chemical Physics, 2015, 143, 094105.	1.2	36
16	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. III. The Covalent Bonding Structure of Urea. Journal of Physical Chemistry A, 2015, 119, 10368-10375.	1.1	37
17	A Comprehensive Analysis in Terms of Molecule-Intrinsic Quasi-Atomic Orbitals. IV. Bond Breaking and Bond Forming along the Dissociative Reaction Path of Dioxetane. Journal of Physical Chemistry A, 2015, 119, 10376-10389.	1.1	31
18	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. II. Strongly Correlated MCSCF Wave Functions. Journal of Physical Chemistry A, 2015, 119, 10360-10367.	1.1	49

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19	Covalent bonds are created by the drive of electron waves to lower their kinetic energy through expansion. Journal of Chemical Physics, 2014, 140, 204104.	1.2	77
20	Accurate ab initio potential energy curves and spectroscopic properties of the four lowest singlet states of C2. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	37
21	In memoriam Hermann Hartmann, founder of TCA, on the occasion of his 100th birthday. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	1
22	A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions. Journal of Chemical Physics, 2013, 139, 234107.	1.2	83
23	Three Millennia of Atoms and Molecules. ACS Symposium Series, 2013, , 1-45.	0.5	9
24	Accurate Potential Energy Curve for B₂. Ab Initio Elucidation of the Experimentally Elusive Ground State Rotation-Vibration Spectrum. Journal of Physical Chemistry A, 2012, 116, 1717-1729.	1.1	23
25	The dispersion interaction between quantum mechanics and effective fragment potential molecules. Journal of Chemical Physics, 2012, 136, 244107.	1.2	29
26	Accurate ab initio potential energy curve of O2. I. Nonrelativistic full configuration interaction valence correlation by the correlation energy extrapolation by intrinsic scaling method. Journal of Chemical Physics, 2010, 132, 074109.	1.2	32
27	A priori identification of configurational deadwood. Chemical Physics, 2009, 356, 64-75.	0.9	65
28	Ab initio potential energy curve of F2. IV. Transition from the covalent to the van der Waals region: Competition between multipolar and correlation forces. Journal of Chemical Physics, 2009, 130, 204101.	1.2	39
29	Physical Understanding through Variational Reasoning: Electron Sharing and Covalent Bonding. Journal of Physical Chemistry A, 2009, 113, 1954-1968.	1.1	61
30	Intrinsic local constituents of molecular electronic wave functions. I. Exact representation of the density matrix in terms of chemically deformed and oriented atomic minimal basis set orbitals. Theoretical Chemistry Accounts, 2008, 120, 281-294.	0.5	44
31	Intrinsic local constituents of molecular electronic wave functions. II. Electronic structure analyses in terms of intrinsic oriented quasi-atomic molecular orbitals for the molecules FOOH, H2BH2BH2, H2CO and the isomerization HNO â†' NOH. Theoretical Chemistry Accounts, 2008, 120, 295-305.	0.5	23
32	Why does electron sharing lead to covalent bonding? A variational analysis. Journal of Computational Chemistry, 2007, 28, 391-410.	1.5	88
33	Accurate ab initio potential energy curve of F2. I. Nonrelativistic full valence configuration interaction energies using the correlation energy extrapolation by intrinsic scaling method. Journal of Chemical Physics, 2007, 127, 164317.	1.2	61
34	Correlation energy extrapolation by intrinsic scaling. IV. Accurate binding energies of the homonuclear diatomic molecules carbon, nitrogen, oxygen, and fluorine. Journal of Chemical Physics, 2005, 122, 154110.	1.2	97
35	Correlation energy extrapolation by intrinsic scaling. II. The water and the nitrogen molecule. Journal of Chemical Physics, 2004, 121, 10919.	1.2	42
36	Correlation energy extrapolation by intrinsic scaling. I. Method and application to the neon atom. Journal of Chemical Physics, 2004, 121, 10905.	1.2	52

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37	Split-localized orbitals can yield stronger configuration interaction convergence than natural orbitals. Journal of Chemical Physics, 2003, 119, 8217-8224.	1.2	66
38	Electron pairs, localized orbitals and electron correlation. Molecular Physics, 2002, 100, 757-781.	0.8	28
39	Deadwood in configuration spaces. II. Singles + doubles and singles + doubles + triples + quadruples spaces. Theoretical Chemistry Accounts, 2002, 107, 220-228.	0.5	33
40	Identification of deadwood in configuration spaces through general direct configuration interaction. Theoretical Chemistry Accounts, 2001, 106, 339-351.	0.5	157
41	New parallel optimal-parameter fast multipole method (OPFMM). Journal of Computational Chemistry, 2001, 22, 1484-1501.	1.5	47
42	Oriented Nonspherical Atoms in Crystals Deduced from X-Ray Scattering Data. Helvetica Chimica Acta, 2001, 84, 1907-1942.	1.0	7
43	Orbital transformations and configurational transformations of electronic wavefunctions. Journal of Chemical Physics, 1999, 111, 2910-2920.	1.2	18
44	A local understanding of the quantum chemical geometric phase theorem in terms of diabatic states. Journal of Chemical Physics, 1999, 110, 4208-4212.	1.2	14
45	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. Journal of Chemical Physics, 1999, 111, 8825-8831.	1.2	146
46	Violation of the weak noncrossing rule between totally symmetric closed-shell states in the valence-isoelectronic series O3, S3, SO2, and S2O. Journal of Chemical Physics, 1997, 107, 4307-4317.	1.2	51
47	Determination of diabatic states through enforcement of configurational uniformity. Theoretical Chemistry Accounts, 1997, 97, 47-58.	0.5	143
48	Rotation Matrices for Real Spherical Harmonics. Direct Determination by Recursion. The Journal of Physical Chemistry, 1996, 100, 6342-6347.	2.9	104
49	Gradient fields of potential energy surfaces. Journal of Chemical Physics, 1994, 100, 5836-5848.	1.2	34
50	A simple prediction of approximate transition states on potential energy surfaces. Journal of Chemical Physics, 1994, 101, 2168-2174.	1.2	12
51	Locating transition states by quadratic image gradient descent on potential energy surfaces. Journal of Chemical Physics, 1994, 101, 2157-2167.	1.2	47
52	Potential energy surfaces of carbon dioxide. International Journal of Quantum Chemistry, 1994, 49, 409-427.	1.0	24
53	Quadratic steepest descent on potential energy surfaces. IV. Adaptation to singular Hessians. Journal of Chemical Physics, 1994, 100, 6101-6101.	1.2	11
54	Quadratic steepest descent on potential energy surfaces. I. Basic formalism and quantitative assessment. Journal of Chemical Physics, 1993, 99, 5257-5268.	1.2	70

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55	A quantum chemical determination of diabatic states. Journal of Chemical Physics, 1993, 99, 3799-3803.	1.2	110
56	Quadratic steepest descent on potential energy surfaces. II. Reaction path following without analytic Hessians. Journal of Chemical Physics, 1993, 99, 5269-5275.	1.2	57
57	Quadratic steepest descent on potential energy surfaces. III. Minima seeking along steepest descent lines. Journal of Chemical Physics, 1993, 99, 5276-5280.	1.2	24
58	Strong shifts in diabatic nondynamic electron correlations cause conical intersection between lowâ€lying closedâ€shell adiabatic singlets of like symmetry in ozone. Journal of Chemical Physics, 1993, 99, 3790-3798.	1.2	34
59	Gradient extremals and steepest descent lines on potential energy surfaces. Journal of Chemical Physics, 1993, 98, 9707-9714.	1.2	94
60	Potential energy surfaces of ozone. I. Journal of Chemical Physics, 1991, 94, 8054-8069.	1.2	129
61	Potential energy surfaces near intersections. Journal of Chemical Physics, 1991, 95, 1862-1876.	1.2	442
62	The ring opening of substituted cyclopropylidenes to substituted allenes: the effects of steric and long-range electrostatic interactions. Theoretica Chimica Acta, 1991, 78, 397-416.	0.9	20
63	Elektronendichte, Deformationsdichte und chemische Bindung. Angewandte Chemie, 1989, 101, 605-607.	1.6	12
64	Generation of a full active configuration space basis in terms of symmetry- and spin-adapted antisymmetrized orbital products. International Journal of Quantum Chemistry, 1987, 31, 489-505.	1.0	7
65	Gradient extremals. Theoretica Chimica Acta, 1986, 69, 265-279.	0.9	137
66	Bifurcations and transition states. Theoretica Chimica Acta, 1986, 69, 281-307.	0.9	202
67	Chemical binding and electron correlation in diatomic molecules as described by the FORS model and the FORS-IACC model. Theoretica Chimica Acta, 1985, 68, 69-86.	0.9	26
68	Pictorial representation of three-dimensional electron distributions through a perspective view of contour diagrams in a set of parallel planes. Journal of Computational Chemistry, 1985, 6, 209-215.	1.5	6
69	Intraatomic correlation correction in the FORS model. The Journal of Physical Chemistry, 1985, 89, 2221-2235.	2.9	38
70	Concerted dihydrogen exchange between ethane and ethylene. SCF and FORS calculations of the barrier. Journal of the American Chemical Society, 1982, 104, 960-967.	6.6	66
71	Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model. Chemical Physics, 1982, 71, 41-49.	0.9	467
72	Are atoms sic to molecular electronic wavefunctions? II. Analysis of fors orbitals. Chemical Physics, 1982, 71, 51-64.	0.9	156

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73	Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations. Chemical Physics, 1982, 71, 65-78.	0.9	163
74	Systematic approach to extended even-tempered orbital bases for atomic and molecular calculations. Theoretica Chimica Acta, 1979, 52, 231-251.	0.9	160
75	An approximate relation between orbital SCF energies and total SCF energy in molecules. Journal of Chemical Physics, 1977, 66, 375-376.	1.2	131
76	MCSCF Studies of Chemical Reactions: Natural Reaction Orbitals and Localized Reaction Orbitals. , 1976, , 505-515.		48
77	Evenâ€tempered atomic orbitals. VI. Optimal orbital exponents and optimal contractions of Gaussian primitives for hydrogen, carbon, and oxygen in molecules. Journal of Chemical Physics, 1974, 60, 918-931.	1.2	118
78	Evenâ€tempered atomic orbitals. VII. Theoretical equilibrium geometries and reaction energies for carbon suboxide and other molecules containing carbon, oxygen, and hydrogen. Journal of Chemical Physics, 1974, 60, 932-936.	1.2	14
79	Evenâ€tempered atomic orbitals. III. Economic deployment of Gaussian primitives in expanding atomic SCF orbitals. Journal of Chemical Physics, 1973, 59, 5956-5965.	1.2	103
80	Evenâ€tempered atomic orbitals. V. SCF calculations of trialkali ions with pseudoscaled, nonorthogonal AO bases. Journal of Chemical Physics, 1973, 59, 5978-5991.	1.2	92
81	Evenâ€tempered atomic orbitals. IV. Atomic orbital bases with pseudoscaling capability for molecular calculations. Journal of Chemical Physics, 1973, 59, 5966-5977.	1.2	47
82	Nonorthogonal atomic selfâ€consistent field orbitals. Journal of Chemical Physics, 1973, 59, 5950-5955.	1.2	15
83	Manyâ€Electron Wavefunctions Expanded in Spinâ€Adapted Antisymmetrized Products, and Their Expectation Values. Journal of Chemical Physics, 1972, 57, 2776-2786.	1.2	58
84	Implementing the SAAP Formalism. II. Simultaneous Eigenfunctions of L2 and S2 by Direct Diagonalization. Journal of Chemical Physics, 1972, 57, 2791-2793.	1.2	13
85	Generalization of Euler Angles to Nâ€Dimensional Orthogonal Matrices. Journal of Mathematical Physics, 1972, 13, 528-533.	0.5	55
86	A quadrupolar expansion forr12?1. International Journal of Quantum Chemistry, 1972, 6, 347-352.	1.0	5
87	An expansion for four-center integrals over Slater-type orbitals. International Journal of Quantum Chemistry, 1972, 6, 353-366.	1.0	13
88	Paradoxical Role of the Kineticâ€Energy Operator in the Formation of the Covalent Bond. Journal of Chemical Physics, 1971, 54, 1495-1511.	1.2	187
89	Comment on the Translation of Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1971, 54, 2291-2292.	1.2	6
90	Heteropolar Oneâ€Electron Bond. Journal of Chemical Physics, 1971, 55, 5804-5818.	1.2	51

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91	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. III. Imidogen. Journal of Chemical Physics, 1970, 52, 1206-1227.	1.2	59
92	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. II. Lithium Hydride and Boron Hydride. Journal of Chemical Physics, 1970, 52, 1181-1205.	1.2	86
93	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. I. Theory. Journal of Chemical Physics, 1970, 52, 1174-1180.	1.2	72
94	The Origin of Binding and Antibinding in the Hydrogen Molecule-Ion. Advances in Quantum Chemistry, 1970, 5, 27-98.	0.4	82
95	Compact natural orbital expansions for the helium ground state. International Journal of Quantum Chemistry, 1969, 3, 107-113.	1.0	12
96	Expansion ofr12 andr12?1 in terms of analytical functions. International Journal of Quantum Chemistry, 1969, 3, 493-501.	1.0	9
97	Twoâ€Center Exchange Integrals between Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1969, 50, 2575-2580.	1.2	45
98	Parametrization of an orthogonal matrix in terms of generalized eulerian angles. International Journal of Quantum Chemistry, 1969, 4, 625-634.	1.0	13
99	Coulomb Integrals over Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1968, 49, 4306-4311.	1.2	35
100	New Aspects of the Bipolar Expansion and Molecular Multicenter Integrals. Journal of Chemical Physics, 1968, 49, 4293-4300.	1.2	34
101	Overlap Integrals over Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1968, 49, 4301-4305.	1.2	41
102	Electron Correlation and Augmented Separatedâ€Pair Expansion in Berylliumlike Atomic Systems. Journal of Chemical Physics, 1968, 48, 3450-3464.	1.2	27
103	Electron Correlation and Augmented Separatedâ€Pair Expansion. Journal of Chemical Physics, 1968, 48, 3444-3449.	1.2	33
104	Quantitative Correlations between Rotational and Vibrational Spectroscopic Constants in Diatomic Molecules. Journal of Chemical Physics, 1968, 49, 5399-5415.	1.2	70
105	Hybrid Integrals over Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1968, 49, 4285-4292.	1.2	32
106	Twoâ€Center Hybrid Integrals between Slaterâ€Type Atomic Orbitals. Journal of Chemical Physics, 1967, 47, 1855-1856.	1.2	5
107	Twoâ€Center Coulomb Integrals between Atomic Orbitals. Journal of Mathematical Physics, 1966, 7, 547-559.	0.5	44
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109	Localized Atomic and Molecular Orbitals. II. Journal of Chemical Physics, 1965, 43, S97-S116.	1.2	300
110	Chemical Binding in the Water Molecule1a. The Journal of Physical Chemistry, 1964, 68, 1628-1653.	2.9	42
111	Localized Atomic and Molecular Orbitals. Reviews of Modern Physics, 1963, 35, 457-464.	16.4	1,423
112	The Physical Nature of the Chemical Bond. Reviews of Modern Physics, 1962, 34, 326-376.	16.4	805
113	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. IV. Integral Formulas. Journal of Chemical Physics, 1961, 34, 1892-1896.	1.2	29
114	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. III. Topological Matrix as Generatrix of Bond Orders. Journal of Chemical Physics, 1961, 34, 1884-1891.	1.2	68
115	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. I. General Analysis in the Tightâ€Binding Formulation. Journal of Chemical Physics, 1961, 34, 1861-1877.	1.2	116
116	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. VI. Theoretical Evaluation of Energy Contributions. Journal of Chemical Physics, 1961, 34, 1907-1913.	1.2	11
117	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. V. Empirical Determination of Integrals between Carbon Atomic Orbitals from Experimental Data on Benzene. Journal of Chemical Physics, 1961, 34, 1897-1907.	1.2	14
118	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. II. Augmented Tightâ€Binding Formulation. Journal of Chemical Physics, 1961, 34, 1878-1883.	1.2	21