

Klaus Ruedenberg

List of Publications by Year in descending order

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118
papers

9,969
citations

53939

47
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39744

98
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127
all docs

127
docs citations

127
times ranked

4503
citing authors

#	ARTICLE	IF	CITATIONS
1	Localized Atomic and Molecular Orbitals. Reviews of Modern Physics, 1963, 35, 457-464.	16.4	1,423
2	The Physical Nature of the Chemical Bond. Reviews of Modern Physics, 1962, 34, 326-376.	16.4	805
3	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
4	Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model. Chemical Physics, 1982, 71, 41-49.	0.9	467
5	Potential energy surfaces near intersections. Journal of Chemical Physics, 1991, 95, 1862-1876.	1.2	442
6	Localized Atomic and Molecular Orbitals. II. Journal of Chemical Physics, 1965, 43, S97-S116.	1.2	300
7	Bifurcations and transition states. Theoretica Chimica Acta, 1986, 69, 281-307.	0.9	202
8	Paradoxical Role of the Kinetic Energy Operator in the Formation of the Covalent Bond. Journal of Chemical Physics, 1971, 54, 1495-1511.	1.2	187
9	Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations. Chemical Physics, 1982, 71, 65-78.	0.9	163
10	Systematic approach to extended even-tempered orbital bases for atomic and molecular calculations. Theoretica Chimica Acta, 1979, 52, 231-251.	0.9	160
11	Identification of deadwood in configuration spaces through general direct configuration interaction. Theoretical Chemistry Accounts, 2001, 106, 339-351.	0.5	157
12	Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of fors orbitals. Chemical Physics, 1982, 71, 51-64.	0.9	156
13	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. Journal of Chemical Physics, 1999, 111, 8825-8831.	1.2	146
14	Determination of diabatic states through enforcement of configurational uniformity. Theoretical Chemistry Accounts, 1997, 97, 47-58.	0.5	143
15	Gradient extremals. Theoretica Chimica Acta, 1986, 69, 265-279.	0.9	137
16	An approximate relation between orbital SCF energies and total SCF energy in molecules. Journal of Chemical Physics, 1977, 66, 375-376.	1.2	131
17	Potential energy surfaces of ozone. I. Journal of Chemical Physics, 1991, 94, 8054-8069.	1.2	129
18	Even-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

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19	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. I. General Analysis in the Tight-Binding Formulation. <i>Journal of Chemical Physics</i> , 1961, 34, 1861-1877.	1.2	116
20	A quantum chemical determination of diabatic states. <i>Journal of Chemical Physics</i> , 1993, 99, 3799-3803.	1.2	110
21	Rotation Matrices for Real Spherical Harmonics. Direct Determination by Recursion. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6342-6347.	2.9	104
22	Even-tempered atomic orbitals. III. Economic deployment of Gaussian primitives in expanding atomic SCF orbitals. <i>Journal of Chemical Physics</i> , 1973, 59, 5956-5965.	1.2	103
23	Correlation energy extrapolation by intrinsic scaling. IV. Accurate binding energies of the homonuclear diatomic molecules carbon, nitrogen, oxygen, and fluorine. <i>Journal of Chemical Physics</i> , 2005, 122, 154110.	1.2	97
24	Gradient extremals and steepest descent lines on potential energy surfaces. <i>Journal of Chemical Physics</i> , 1993, 98, 9707-9714.	1.2	94
25	Even-tempered atomic orbitals. V. SCF calculations of trialkali ions with pseudoscaled, nonorthogonal AO bases. <i>Journal of Chemical Physics</i> , 1973, 59, 5978-5991.	1.2	92
26	Why does electron sharing lead to covalent bonding? A variational analysis. <i>Journal of Computational Chemistry</i> , 2007, 28, 391-410.	1.5	88
27	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. II. Lithium Hydride and Boron Hydride. <i>Journal of Chemical Physics</i> , 1970, 52, 1181-1205.	1.2	86
28	A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions. <i>Journal of Chemical Physics</i> , 2013, 139, 234107.	1.2	83
29	The Origin of Binding and Antibinding in the Hydrogen Molecule-Ion. <i>Advances in Quantum Chemistry</i> , 1970, 5, 27-98.	0.4	82
30	Covalent bonds are created by the drive of electron waves to lower their kinetic energy through expansion. <i>Journal of Chemical Physics</i> , 2014, 140, 204104.	1.2	77
31	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. I. Theory. <i>Journal of Chemical Physics</i> , 1970, 52, 1174-1180.	1.2	72
32	Quantitative Correlations between Rotational and Vibrational Spectroscopic Constants in Diatomic Molecules. <i>Journal of Chemical Physics</i> , 1968, 49, 5399-5415.	1.2	70
33	Quadratic steepest descent on potential energy surfaces. I. Basic formalism and quantitative assessment. <i>Journal of Chemical Physics</i> , 1993, 99, 5257-5268.	1.2	70
34	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. III. Topological Matrix as Generatrix of Bond Orders. <i>Journal of Chemical Physics</i> , 1961, 34, 1884-1891.	1.2	68
35	Concerted dihydrogen exchange between ethane and ethylene. SCF and FORS calculations of the barrier. <i>Journal of the American Chemical Society</i> , 1982, 104, 960-967.	6.6	66
36	Split-localized orbitals can yield stronger configuration interaction convergence than natural orbitals. <i>Journal of Chemical Physics</i> , 2003, 119, 8217-8224.	1.2	66

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37	A priori identification of configurational deadwood. <i>Chemical Physics</i> , 2009, 356, 64-75.	0.9	65
38	Accurate <i>ab initio</i> potential energy curve of F ₂ . I. Nonrelativistic full valence configuration interaction energies using the correlation energy extrapolation by intrinsic scaling method. <i>Journal of Chemical Physics</i> , 2007, 127, 164317.	1.2	61
39	Physical Understanding through Variational Reasoning: Electron Sharing and Covalent Bonding. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1954-1968.	1.1	61
40	Electron Correlation and Separated Pair Approximation in Diatomic Molecules. III. Imidogen. <i>Journal of Chemical Physics</i> , 1970, 52, 1206-1227.	1.2	59
41	Many-Electron Wavefunctions Expanded in Spin-Adapted Antisymmetrized Products, and Their Expectation Values. <i>Journal of Chemical Physics</i> , 1972, 57, 2776-2786.	1.2	58
42	Quadratic steepest descent on potential energy surfaces. II. Reaction path following without analytic Hessians. <i>Journal of Chemical Physics</i> , 1993, 99, 5269-5275.	1.2	57
43	Generalization of Euler Angles to N-Dimensional Orthogonal Matrices. <i>Journal of Mathematical Physics</i> , 1972, 13, 528-533.	0.5	55
44	Correlation energy extrapolation by intrinsic scaling. I. Method and application to the neon atom. <i>Journal of Chemical Physics</i> , 2004, 121, 10905.	1.2	52
45	Heteropolar One-Electron Bond. <i>Journal of Chemical Physics</i> , 1971, 55, 5804-5818.	1.2	51
46	Violation of the weak noncrossing rule between totally symmetric closed-shell states in the valence-isoelectronic series O ₃ , S ₃ , SO ₂ , and S ₂ O. <i>Journal of Chemical Physics</i> , 1997, 107, 4307-4317.	1.2	51
47	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. II. Strongly Correlated MCSCF Wave Functions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10360-10367.	1.1	49
48	MCSCF Studies of Chemical Reactions: Natural Reaction Orbitals and Localized Reaction Orbitals. , 1976, , 505-515.		48
49	Even-tempered atomic orbitals. IV. Atomic orbital bases with pseudoscaling capability for molecular calculations. <i>Journal of Chemical Physics</i> , 1973, 59, 5966-5977.	1.2	47
50	Locating transition states by quadratic image gradient descent on potential energy surfaces. <i>Journal of Chemical Physics</i> , 1994, 101, 2157-2167.	1.2	47
51	New parallel optimal-parameter fast multipole method (OPFMM). <i>Journal of Computational Chemistry</i> , 2001, 22, 1484-1501.	1.5	47
52	Two-Center Exchange Integrals between Slater-Type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1969, 50, 2575-2580.	1.2	45
53	Two-Center Coulomb Integrals between Atomic Orbitals. <i>Journal of Mathematical Physics</i> , 1966, 7, 547-559.	0.5	44
54	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. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 281-294.	0.5	44

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55	Intrinsic Resolution of Molecular Electronic Wave Functions and Energies in Terms of Quasi-atoms and Their Interactions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1086-1105.	1.1	44
56	The Virial Theorem and Covalent Bonding. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7880-7893.	1.1	43
57	Chemical Binding in the Water Molecule. <i>The Journal of Physical Chemistry</i> , 1964, 68, 1628-1653.	2.9	42
58	Correlation energy extrapolation by intrinsic scaling. II. The water and the nitrogen molecule. <i>Journal of Chemical Physics</i> , 2004, 121, 10919.	1.2	42
59	Overlap Integrals over Slater-type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1968, 49, 4301-4305.	1.2	41
60	<i>Ab initio</i> potential energy curve of F ₂ . IV. Transition from the covalent to the van der Waals region: Competition between multipolar and correlation forces. <i>Journal of Chemical Physics</i> , 2009, 130, 204101.	1.2	39
61	Intraatomic correlation correction in the FORS model. <i>The Journal of Physical Chemistry</i> , 1985, 89, 2221-2235.	2.9	38
62	Accurate <i>ab initio</i> potential energy curves and spectroscopic properties of the four lowest singlet states of C ₂ . <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	37
63	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. III. The Covalent Bonding Structure of Urea. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10368-10375.	1.1	37
64	Seniority number description of potential energy surfaces: Symmetric dissociation of water, N ₂ , C ₂ , and Be ₂ . <i>Journal of Chemical Physics</i> , 2015, 143, 094105.	1.2	36
65	Coulomb Integrals over Slater-type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1968, 49, 4306-4311.	1.2	35
66	New Aspects of the Bipolar Expansion and Molecular Multicenter Integrals. <i>Journal of Chemical Physics</i> , 1968, 49, 4293-4300.	1.2	34
67	Strong shifts in diabatic nondynamic electron correlations cause conical intersection between low-lying closed-shell adiabatic singlets of like symmetry in ozone. <i>Journal of Chemical Physics</i> , 1993, 99, 3790-3798.	1.2	34
68	Gradient fields of potential energy surfaces. <i>Journal of Chemical Physics</i> , 1994, 100, 5836-5848.	1.2	34
69	Electron Correlation and Augmented Separated-Pair Expansion. <i>Journal of Chemical Physics</i> , 1968, 48, 3444-3449.	1.2	33
70	Deadwood in configuration spaces. II. Singles + doubles and singles + doubles + triples + quadruples spaces. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 220-228.	0.5	33
71	Hybrid Integrals over Slater-type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1968, 49, 4285-4292.	1.2	32
72	Accurate <i>ab initio</i> potential energy curve of O ₂ . I. Nonrelativistic full configuration interaction valence correlation by the correlation energy extrapolation by intrinsic scaling method. <i>Journal of Chemical Physics</i> , 2010, 132, 074109.	1.2	32

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73	A Comprehensive Analysis in Terms of Molecule-Intrinsic Quasi-Atomic Orbitals. IV. Bond Breaking and Bond Forming along the Dissociative Reaction Path of Dioxetane. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10376-10389.	1.1	31
74	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. IV. Integral Formulas. <i>Journal of Chemical Physics</i> , 1961, 34, 1892-1896.	1.2	29
75	The dispersion interaction between quantum mechanics and effective fragment potential molecules. <i>Journal of Chemical Physics</i> , 2012, 136, 244107.	1.2	29
76	Electron Correlation and Electron- σ -Pair Wavefunction for the Beryllium Atom. <i>Journal of Chemical Physics</i> , 1965, 43, S88-S90.	1.2	28
77	Electron pairs, localized orbitals and electron correlation. <i>Molecular Physics</i> , 2002, 100, 757-781.	0.8	28
78	Electron Correlation and Augmented Separated- σ -Pair Expansion in Berylliumlike Atomic Systems. <i>Journal of Chemical Physics</i> , 1968, 48, 3450-3464.	1.2	27
79	Chemical binding and electron correlation in diatomic molecules as described by the FORS model and the FORS-IACC model. <i>Theoretica Chimica Acta</i> , 1985, 68, 69-86.	0.9	26
80	Quadratic steepest descent on potential energy surfaces. III. Minima seeking along steepest descent lines. <i>Journal of Chemical Physics</i> , 1993, 99, 5276-5280.	1.2	24
81	Potential energy surfaces of carbon dioxide. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 409-427.	1.0	24
82	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, H ₂ BH ₂ BH ₂ , H ₂ CO and the isomerization HNO \rightarrow NOH. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 295-305.	0.5	23
83	Accurate Potential Energy Curve for B ₂ . Ab Initio Elucidation of the Experimentally Elusive Ground State Rotation-Vibration Spectrum. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1717-1729.	1.1	23
84	Correlation Energy Extrapolation by Many-Body Expansion. <i>Journal of Physical Chemistry A</i> , 2017, 121, 836-844.	1.1	23
85	Dispersion Interactions in QM/EFP. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9495-9507.	1.1	23
86	Identification and Characterization of Molecular Bonding Structures by ab initio Quasi-Atomic Orbital Analyses. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8884-8898.	1.1	23
87	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. II. Augmented Tight-Binding Formulation. <i>Journal of Chemical Physics</i> , 1961, 34, 1878-1883.	1.2	21
88	The ring opening of substituted cyclopropylidenes to substituted allenes: the effects of steric and long-range electrostatic interactions. <i>Theoretica Chimica Acta</i> , 1991, 78, 397-416.	0.9	20
89	Why is Si ₂ H ₂ Not Linear? An Intrinsic Quasi-Atomic Bonding Analysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 13729-13742.	6.6	19
90	Orbital transformations and configurational transformations of electronic wavefunctions. <i>Journal of Chemical Physics</i> , 1999, 111, 2910-2920.	1.2	18

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91	Relativistic <i>ab Initio</i> Accurate Atomic Minimal Basis Sets: Quantitative LUMOs and Oriented Quasi-Atomic Orbitals for the Elements Li–Xe. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3588-3597.	1.1	18
92	Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3442-3454.	1.1	18
93	Quasi-Atomic Bond Analyses in the Sixth Period: II. Bond Analyses of Cerium Oxides. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5249-5256.	1.1	18
94	Multiple Bonding in Rhodium Monoboride. Quasi-atomic Analyses of the Ground and Low-Lying Excited States. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4836-4846.	1.1	16
95	Nonorthogonal atomic self-consistent field orbitals. <i>Journal of Chemical Physics</i> , 1973, 59, 5950-5955.	1.2	15
96	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. V. Empirical Determination of Integrals between Carbon Atomic Orbitals from Experimental Data on Benzene. <i>Journal of Chemical Physics</i> , 1961, 34, 1897-1907.	1.2	14
97	Even-tempered atomic orbitals. VII. Theoretical equilibrium geometries and reaction energies for carbon suboxide and other molecules containing carbon, oxygen, and hydrogen. <i>Journal of Chemical Physics</i> , 1974, 60, 932-936.	1.2	14
98	A local understanding of the quantum chemical geometric phase theorem in terms of diabatic states. <i>Journal of Chemical Physics</i> , 1999, 110, 4208-4212.	1.2	14
99	Implementing the SAAP Formalism. II. Simultaneous Eigenfunctions of L2 and S2 by Direct Diagonalization. <i>Journal of Chemical Physics</i> , 1972, 57, 2791-2793.	1.2	13
100	An expansion for four-center integrals over Slater-type orbitals. <i>International Journal of Quantum Chemistry</i> , 1972, 6, 353-366.	1.0	13
101	Parametrization of an orthogonal matrix in terms of generalized eulerian angles. <i>International Journal of Quantum Chemistry</i> , 1969, 4, 625-634.	1.0	13
102	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. <i>Journal of Chemical Physics</i> , 2016, 144, 104304.	1.2	13
103	Compact natural orbital expansions for the helium ground state. <i>International Journal of Quantum Chemistry</i> , 1969, 3, 107-113.	1.0	12
104	Elektronendichte, Deformationsdichte und chemische Bindung. <i>Angewandte Chemie</i> , 1989, 101, 605-607.	1.6	12
105	A simple prediction of approximate transition states on potential energy surfaces. <i>Journal of Chemical Physics</i> , 1994, 101, 2168-2174.	1.2	12
106	Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. VI. Theoretical Evaluation of Energy Contributions. <i>Journal of Chemical Physics</i> , 1961, 34, 1907-1913.	1.2	11
107	Quadratic steepest descent on potential energy surfaces. IV. Adaptation to singular Hessians. <i>Journal of Chemical Physics</i> , 1994, 100, 6101-6101.	1.2	11
108	Quasi-Atomic Bond Analyses in the Sixth Period: I. Relativistic Accurate Atomic Minimal Basis Sets for the Elements Cesium to Radon. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5242-5248.	1.1	11

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109	Expansion of $12\text{-}r$ and $12\text{-}r^2$ in terms of analytical functions. <i>International Journal of Quantum Chemistry</i> , 1969, 3, 493-501.	1.0	9
110	Three Millennia of Atoms and Molecules. <i>ACS Symposium Series</i> , 2013, , 1-45.	0.5	9
111	Atoms and interatomic bonding synergism inherent in molecular electronic wave functions. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	9
112	Generation of a full active configuration space basis in terms of symmetry- and spin-adapted antisymmetrized orbital products. <i>International Journal of Quantum Chemistry</i> , 1987, 31, 489-505.	1.0	7
113	Oriented Nonspherical Atoms in Crystals Deduced from X-Ray Scattering Data. <i>Helvetica Chimica Acta</i> , 2001, 84, 1907-1942.	1.0	7
114	Comment on the Translation of Slater-type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1971, 54, 2291-2292.	1.2	6
115	Pictorial representation of three-dimensional electron distributions through a perspective view of contour diagrams in a set of parallel planes. <i>Journal of Computational Chemistry</i> , 1985, 6, 209-215.	1.5	6
116	Two-Center Hybrid Integrals between Slater-type Atomic Orbitals. <i>Journal of Chemical Physics</i> , 1967, 47, 1855-1856.	1.2	5
117	A quadrupolar expansion for $12\text{-}r$. <i>International Journal of Quantum Chemistry</i> , 1972, 6, 347-352.	1.0	5
118	In memoriam Hermann Hartmann, founder of TCA, on the occasion of his 100th birthday. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	1