

Publications of Klaus Ruedenberg, 1951 - 2022

- (1) On the Theory of Strong Coupling between Nucleons and Pseudovector Mesons, K. Ruedenberg, *Helvetica Physica Acta*, 24, 89-136 (1951).
- (2) A Mobile Electron Model for Aromatic Molecules, K. Ruedenberg and R. G. Parr, *J. Chem. Phys.*, 19, 1268-1271 (1951).
- (3) A Study of the Two-Center Exchange Integrals in Molecular Problems, K. Ruedenberg, *J. Chem. Phys.*, 19, 1459-1477 (1951).
- (4) A Note on the Three- and Four-Center Integrals in Molecular Problems, K. Ruedenberg, *J. Chem. Phys.*, 19, 1433 (1951)
- (5) Progress Report on the Investigation of Integrals between Slater Atomic Orbitals and their Application in Molecular Calculations, K. Ruedenberg, Technical Report 1952-1953, Part Two, Pages xiv – xxi (Laboratory of Molecular Structure and Spectra, Department of Physics, The University of Chicago, 1953).
- (6) Free-Electron Network Model for Conjugated Systems. I. Theory, K. Ruedenberg and C. W. Scherr, *J. Chem. Phys.*, 21, 1565-1581 (1953).
- (7) Free-Electron Network Model for Conjugated Systems. V. Theoretical Equivalence with the LCAO MO Model, K. Ruedenberg, *J. Chem. Phys.*, 22, 1878-1895 (1954).
- (8) A Study of the Two-Center Hybrid Integrals and a Unified Treatment of the Hybrid, Coulomb, and One-Electron Integrals, K. Ruedenberg, C. C. J. Roothaan and W. Jaunzemis, *J. Chem. Phys.*, 24, 201-220 (1956).
- (9) Electronic Interaction in the Free-Electron Network Model for Conjugated Systems. I. Theory, N. S. Ham and K. Ruedenberg, *J. Chem. Phys.*, 25, 1-13 (1956).
- (10) Electronic Interaction in the Free-Electron Network Model for Conjugated Systems. II. Spectra of Aromatic Hydrocarbons, N. S. Ham and K. Ruedenberg, *J. Chem. Phys.*, 25, 13-26 (1956).
- (11) Energy Levels, Atom Populations, Bond Populations in the LCAO MO Model and in the FE MO Model. A Quantitative Analysis, N. S. Ham and K. Ruedenberg, *J. Chem. Phys.*, 29, 1199-1214 (1958).
- (12) Mobile Bond Orders in Conjugated Systems, N. S. Ham and K. Ruedenberg, *J. Chem. Phys.*, 29, 1215-1222 (1958).
- (13) Theorem on the Mobile Bond Orders of Alternant Conjugated Systems, K. Ruedenberg, *J.*

Chem. Phys., 29, 1232-1234 (1958).

(14) Boulder Conference on Molecular Quantum Mechanics, K. Ruedenberg, *Physics Today*, 13, 5, 34-36 (1960).

(15) Spectral Characteristics of Several Series of More Unusual Aromatic Hydrocarbons, E. Miller Layton, Jr., *J. Mol. Spectroscopy* 5, 181 (1960). Directed by K. Ruedenberg.

(16) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. I. General Analysis of the Tight-Binding Approximation, K. Ruedenberg, *J. Chem. Phys.*, 34, 1861-1878 (1961).

(17) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. II. Augmented Tight-Binding Approximation, K. Ruedenberg, *J. Chem. Phys.*, 34, 1878-1884 (1961).

(18) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. III. Topological Matrix as Generatrix of Bond Orders, K. Ruedenberg, *J. Chem. Phys.*, 34, 1884-1892 (1961).

(19) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. IV. Integral Formulas, K. Ruedenberg, *J. Chem. Phys.*, 34, 1892-1897 (1961)

(20) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. V. Empirical Determination of Integrals between Carbon Atomic Orbitals from Experimental Data on Benzene, K. Ruedenberg and E. M. Layton, Jr., *J. Chem. Phys.*, 34, 1897-1907 (1961).

(21) Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. VI. Theoretical Evaluation of Energy Contributions, K. Ruedenberg, *J. Chem. Phys.*, 34, 1907-1917 (1961).

(22) The Physical Nature of the Chemical Bond. K. Ruedenberg, *Revs. Modern Phys.*, 34, 326-376 (1962).

(23) Ligand Field Theory of Square-Planar Platinum(II) Complexes, R. F. Fenske, D. S. Martin and K. Ruedenberg, *Inorganic Chem.*, 1, 441-452 (1962).

(24) Electronic Structure and Spectra of Conjugated Hydrocarbons, R. L. Hummel and K. Ruedenberg, *J. Phys. Chem.*, 66, 2334-2359 (1962).

(25) Calculation on Electronic Spectra of Catacondensed and Pericondensed Aromatic Hydrocarbons, R. L. Hummel and K. Ruedenberg, USAEC Research and Development Report, No. IS-450 (Office of Technical Services, U.S. Department of Commerce, Washington, D.C., 1964).

(26) Localized Atomic and Molecular Orbitals, C. Edmiston and K. Ruedenberg, *Revs. Modern Phys.*, 35, 457-465 (1963).

(27) Two-Center Electron Interaction Energies, K. Ruedenberg, in "Molecular Orbitals in Chemistry, Physics and Biology". Edited by P. O. Löwdin and B. Pullman (Academic Press,

1964) pp. 215-225.

(28) Hindered Rotation, Hellmann-Feynman Theorem, and Localized Molecular Orbitals, K. Ruedenberg, *J. Chem. Phys.*, 41, 588 (1964).

(29) Chemical Binding in the Water Molecule, C. Edmiston and K. Ruedenberg, *J. Phys. Chem.*, 68, 1628-1653 (1964).

(30) Chemical Binding in Diatomic Hydrides, E. M. Layton, Jr. and K. Ruedenberg, *J. Phys. Chem.*, 68, 1654-1676 (1964).

(31) Chemical Binding in Homonuclear Diatomics, R. R. Rue and K. Ruedenberg, *J. Phys. Chem.*, 68, 1676-1704 (1964).

(32) Deviations from the Virial Relationship in Many-Centered Variational Functions, Allen L. Wasserman, *J. Chem. Phys.* 40, 1812-1814 (1964). Under direction of K. Ruedenberg.

(33) Free-Electron Network for Conjugated Systems. VII. A Note on the Joint Condition, K. Ruedenberg, in "Free-Electron Theory of Conjugated Molecules" (Wiley and Sons, 1964) Section 8.

(34) Book: "Free-Electron Theory of Conjugated Molecules" by J. R. Platt, K. Ruedenberg, C. W. Scherr, N. S. Ham, H. Labhart and W. Lichten (Wiley, 1964). (Contains items No. 5,6,8,9,10,11,12,16,30 of present publication list).

(35) Book: "The Physical Nature of the Chemical Bond" by K. Ruedenberg (MIR Publishing House, Moscow, 1964). (Unauthorized paperback edition of unauthorized Russian translation of item No. 20 of present publication list).

(36) Three-Dimensional and One-Dimensional Free-Electron Molecular Orbitals, R. L. Hummel and K. Ruedenberg, *Istanbul Lectures on Quantum Chemistry*, Edited by O. Sinanoglu (Academic Press 1965) Vol. 1, p. 113-123.

(37) Localized Self-Consistent-Field Orbitals in Atoms and Molecules, K. Ruedenberg, *Istanbul Lectures on Quantum Chemistry*, Edited by O. Sinanoglu (Academic Press, 1965) Vol. 1, p. 85-100.

(38) Localized Atomic and Molecular Orbitals. II, C. Edmiston and K. Ruedenberg, *J. Chem. Phys.*, 43, S97-S115 (1965).

(39) Electron Correlation and Electron Pair Wavefunction for the Beryllium Atom, K. Miller and K. Ruedenberg, *J. Chem. Phys.*, 43, S88-S90 (1965).

(40) Overlap Integrals between Atomic Orbitals, K. Ruedenberg, K. Oohata and D. Wilson, *J. Math. Phys.*, 7, 539-546 (1966).

- (41) Two-Center Coulomb Integrals between Atomic Orbitals, Kiyosi Oohata and Klaus Ruedenberg, *J. Math. Phys.*, 7, 547-559 (1966).
- (42) Localized Atomic and Molecular Orbitals. III, C. Edmiston and K. Ruedenberg, *Quantum Theory of Atoms, Molecules and the Solid State* (P. O. Löwdin, Editor, Academic Press, 1966) p. 263-280.
- (43) Robert S. Mulliken, Nobelpreisträger für Chemie 1966, Klaus Ruedenberg, *Neue Zürcher Zeitung*, Vol. 187, No. 4937, p. 1 (November 16, 1966).
- (44) Bipolare Entwicklungen, Fourier Transformation und Molekulare Mehrzentren-Integrale, K. Ruedenberg, *Theor. Chim. Acta*, 7, 359-366 (1967).
- (45) Two-Center Hybrid Integrals between Slater-Type Atomic Orbitals, R. E. Christoffersen and K. Ruedenberg, *J. Chem. Phys.*, 47, 1855-1856 (1967).
- (46) Electron Correlation and Separated Pair Approximation in Beryllium-like Atomic Systems, K. J. Miller and K. Ruedenberg, *J. Chem. Phys.*, 48, 3414-3443 (1968).
- (47) Electron Correlation and the Augmented Separated Pair Approximation, K. J. Miller and K. Ruedenberg, *J. Chem. Phys.*, 48, 3444-3449 (1968).
- (48) Electron Correlation and Augmented Separated Pair Approximation in Beryllium-like Atomic Systems, K. J. Miller and K. Ruedenberg, *J. Chem. Phys.*, 48, 3450-3464 (1968).
- (49) Analysis and Evaluation of Two-Center Hybrid Integrals over Slater-Type Atomic Orbitals, R. E. Christoffersen and K. Ruedenberg, *J. Chem. Phys.*, 49, 4285-4292 (1968).
- (50) Atomic Orbital Overlap Integrals, D. M. Silver and K. Ruedenberg, *J. Chem. Phys.*, 49, 4301-4305 (1968).
- (51) Coulomb Integrals between Slater-Type Atomic Orbitals, D. M. Silver and K. Ruedenberg, *J. Chem. Phys.*, 49, 4306-4311 (1968).
- (52) A New Form of the Bipolar Expansion and Molecular Multicenter Integrals, L. S. Salmon, F. W. Birss, K. Ruedenberg, *J. Chem. Phys.*, 49, 4293-4300 (1968).
- (53) Two-Centered Coulomb and Hybrid Integrals, K. J. Miller, *J. Math. Phys.* 9, 1292-1294 (1968). Under supervision of K. Ruedenberg.
- (54) Accurate Correlations between Rotational and Vibrational Spectroscopic Constants in Diatomic Molecules, G. V. Calder and K. Ruedenberg, *J. Chem. Phys.*, 49, 5399-5415 (1968).
- (55) Two-Center Exchange Integrals between Slater-Type Atomic Orbitals, E. L. Mehler and K. Ruedenberg, *J. Chem. Phys.*, 50, 2575-2580 (1969).

- (56) Compact Natural Orbital Expansions of the Helium Ground State, N. Cressy, K. J. Miller and K. Ruedenberg, *Intern. Journal of Quantum Chemistry*, 3, 107-113 (1969).
- (57) Expansion of r_{12} and r_{12}^{-1} in Terms of Analytical Functions, N. Cressy and K. Ruedenberg, *Intern. Journal of Quantum Chemistry*, 3, 493-501 (1969).
- (58) Natural Orbital Expansion of Interacting Geminals, D. M. Silver, *J. Chem. Phys.* 50, 5108-5116 (1969). Under supervision of K. Ruedenberg.
- (59) Energy Localization of Approximate Localized Orbitals, W. England and M. S. Gordon, *J. Am. Chem. Soc.* 91, 6864-6866 (1969). Under supervision of K. Ruedenberg.
- (60) Poly-Polar Expansions for Regular and Irregular Spherical Harmonics in Molecules, Otto Steinborn, *Chemical Physics Letters* 3, 671-676 (1969). Under direction of K. Ruedenberg.
- (61) Influence of Long Range Coulombic Interactions on Binding Energy Curves of Molecular Ions, M. J. Feinberg, *Theoretica Chimica Acta* 19, 109-120 (1970). Under supervision of K. Ruedenberg.
- (62) The Origin of Binding and Antibinding in the Hydrogen Molecule Ion, M. J. Feinberg, K. Ruedenberg and E. Mehler, *Advances in Quantum Chemistry*, (P. O. Löwdin, Editor) Vol. 5, pp. 27-98 (Academic Press, 1970).
- (63) Electron Correlation and Separated Pair Approximation in Diatomic Molecules. I. Theory, D. M. Silver, E. L. Mehler, and K. Ruedenberg, *J. Chem. Phys.*, 52, 1174-1180 (1970).
- (64) Electron Correlation and Separated Pair Approximation in Diatomic Molecules. II. Lithium Hydride and Boron Hydride, E. L. Mehler, K. Ruedenberg and D. M. Silver, *J. Chem. Phys.*, 52, 1181-1205 (1970).
- (65) Electron Correlation and Separated Pair Approximation in Diatomic Molecules. III. Imidogen, D. M. Silver, K. Ruedenberg and E. L. Mehler, *J. Chem. Phys.*, 52, 1206-1277 (1970).
- (66) Parametrization of an Orthogonal Matrix, R. Raffenetti and K. Ruedenberg, *Int. J. Quantum Chemistry*, 3S, 625-634 (1970).
- (67) Continuous Degeneracy and Energy Localization of Molecular Orbitals, W. England, *Int. Journ. Quantum Chemistry* 5, 683-697 (1971). Under supervision of K. Ruedenberg.
- (68) Localized Charge Distributions. I. General Theory, Energy Partitioning and the Internal Rotation Barrier in Ethane, W. England and M. S. Gordon, *J. Am. Chem. Soc.* 93, 4649-4657 (1971). Under supervision of K. Ruedenberg.
- (69) Paradoxical Role of the Kinetic Energy Operator in the Formation of the Covalent Bond, M. J. Feinberg and K. Ruedenberg, *J. Chem. Phys.*, 54, 1495-1511 (1971).

- (70) Translation of Slater-Type Atomic Orbitals, W. England and K. Ruedenberg, *J. Chem. Phys.*, 54, 2291 (1971).
- (71) Numerical Analysis and Evaluation of Normalized Repeated Integrals of the Error Function and Related Functions, R. D. Bardo and K. Ruedenberg, *J. of Computational Physics*, 8, 167-174 (1971).
- (72) Localized Molecular Orbitals: A Bridge between Chemical Intuition and Molecular Quantum Mechanics, W. England, L. S. Salmon and K. Ruedenberg, *Fortschritte der Chemischen Forschung (Topics in Current Chemistry)*, 23, 31-123 (1971).
- (73) Localized pi-Orbitals, Pauling Bond Orders and the Origin of Aromatic Stability, W. England and K. Ruedenberg, *Theoretica Chimica Acta*, 22, 196-213 (1971).
- (74) The Heteropolar One-Electron Bond, M. J. Feinberg and K. Ruedenberg, *J. Chem. Phys.*, 55, 5804-5818 (1971).
- (75) Expectation Values of Many-Fermion Spin Eigenstates, K. Ruedenberg, *Phys. Rev. Letters*, 27, 1105-1108 (1971).
- (76) One-Center Coulomb, Two-Center Hybrid and Two-Center Coulomb Integrals for Slater-Transform-Preuss Atomic Orbitals, W. England, *Int. Journ. Quantum Chemistry*, 6, 509-518 (1972). Under supervision of K. Ruedenberg.
- (77) Localized Charge Distributions. II. An Interpretation of the Barriers to Internal Rotation in H₂O₂, W. England and M. S. Gordon, *J. Am. Chem. Soc.* 94, 4818-4823 (1972). Under supervision of K. Ruedenberg.
- (78) Localized Charge Distributions. III. Transferability and Trends of CH Moments and Energies in Acyclic Hydrocarbons, M. S. Gordon and W. England, *J. Am. Chem. Soc.* 94, 5168-5178 (1972). Under supervision of K. Ruedenberg.
- (79) Localized Charge Distributions. IV. The Internal Rotation Barrier in Borazene, M. S. Gordon and W. England, *Chemical Physics Letters* 15, 59-64 (1972). Under supervision of K. Ruedenberg.
- (80) Quadrupolar Expansion for r_{12}^{-1} , L. S. Salmon and K. Ruedenberg, *Int. Journ. Quantum Chemistry*, 6, 347-352 (1972).
- (81) An Expansion for Four-Center Integrals over Slater-Type Atomic Orbitals, L. S. Salmon and K. Ruedenberg, *Int. Journ. Quantum Chemistry*, 6, 353-366 (1972).
- (82) Generalization of Euler Angles to N-Dimensional Orthogonal Matrices, David K. Hoffman, Richard C. Raffanetti and K. Ruedenberg, *J. Mathem. Phys.*, 13, 528-532 (1972).
- (83) Matrix Elements and Density Matrices for Many-Electron Spin Eigenstates Built from

- Orthonormal Orbitals, K. Ruedenberg and R. D. Poshusta, *Advances in Quantum Chemistry* (P. O. Löwdin, Editor) Vol 6, pp. 267-298 (Academic Press, 1972).
- (84) Molecular One-Electron Integrals over Slater-Type Atomic Orbitals and Irregular Solid Spherical Harmonics, E. O. Steinborn and K. Ruedenberg, *Int. Journ. Quantum Chemistry*, 6, 413-438 (1972).
- (85) Many-Electron Wavefunctions Expanded in Spin-Adapted Antisymmetrized Products and Their Expectation Values, W. I. Salmon and K. Ruedenberg, *J. Chem. Phys.*, 57, 2776-2786 (1972).
- (86) Implementing the SAAP Formalism I. Serber-Type Spin Eigenfunctions by Direct Diagonalization, W. I. Salmon, K. Ruedenberg, and L. M. Cheung, *J. Chem. Phys.*, 57, 2787-2790 (1972).
- (87) Implementing the SAAP Formalism II. Simultaneous Eigenfunctions of L² and S² by Direct Diagonalization, W. I. Salmon and K. Ruedenberg, *J. Chem. Phys.*, 57, 2791-2793 (1972).
- (88) Even-Tempered Atomic Orbitals II. Atomic Self-Consistent-Field Wave Functions in Terms of Even-Tempered Exponential Bases, R. C. Raffanetti, *J. Chem. Phys.*, 59, 5936-5950 (1973). Under supervision of K. Ruedenberg.
- (89) Convergence of the Completely Separated Bipolar Expansion of r_{12}^{-1} , L. S. Salmon, *Int. J. Quantum Chemistry* 7, 411-424 (1973). Under supervision of K. Ruedenberg.
- (90) Localized Charge Distributions V. The Internal Rotation Barriers in Methylamine, Methyl Alcohol, Propene and Acetaldehyde, M. S. Gordon and W. England, *J. Am. Chem. Soc.*, 95, 1753-1760 (1973). Under supervision of K. Ruedenberg.
- (91) First Order Scheme for Energy Localization, W. England, *J. Chem. Phys.*, 58, 5182 (1973). Under supervision of K. Ruedenberg.
- (92) Rotation and Translation of Regular and Irregular Solid Spherical Harmonics, E. O. Steinborn and K. Ruedenberg, *Advances in Quantum Chemistry* (P. O. Löwdin, Editor) Vol. 7, 1-81 (1973).
- (93) Molecular Integrals between Real and between Complex Spherical Harmonics, E. O. Steinborn and K. Ruedenberg, *Advances in Quantum Chemistry* (P. O. Löwdin, Editor) Vol. 7, 83-112 (1973).
- (94) Description of Molecules in Terms of Localized Orbitals, K. Ruedenberg, *Computational Methods for Large Molecules and Localized States in Solids* (F. Herman, A. D. McLean, and R. K. Nesbet, Editors; Plenum Press, New York and London, 1973) p. 149-156.
- (95) Even-Tempered Orbital Bases for Atoms and Molecules, K. Ruedenberg, R. C. Raffanetti, R. D. Bardo, *Proceedings of the 1972 Boulder Summer Research Conference on Theoretical*

Chemistry, (Ed. D. W. Smith, Wiley, N. Y., 1973) p. 164.

(96) Nonorthogonal Atomic Self-Consistent-Field Orbitals, R. C. Raffinetti and K. Ruedenberg, *J. Chem. Phys.*, 59, 5950-5955 (1973).

(97) Even-Tempered Atomic Orbitals III. Economic Deployment of Gaussian Primitives in Expanding Atomic SCF Orbitals, R. D. Bardo and K. Ruedenberg, *J. Chem. Phys.*, 59, 5956-5965 (1973).

(98) Even-Tempered Atomic Orbitals IV. Atomic Orbital Bases with Pseudo-Scaling Capability for Molecular Calculations, R. D. Bardo and K. Ruedenberg, *J. Chem. Phys.*, 59, 5966-5977 (1973).

(99) Even-Tempered Atomic Orbitals V. SCF Calculations of Trialkali Ions with Pseudo-scaled Non-Orthogonal Bases, R. C. Raffinetti and K. Ruedenberg, *J. Chem. Phys.*, 59, 5978-5991 (1973).

(100) Even-Tempered Exponential Representations of Atomic Self-Consistent-Field Wavefunctions, R. C. Raffinetti and K. Ruedenberg, USAEC Research and Development Report No. 1S 3195, Ames Laboratory, USAEC, Iowa State University, September 1973.

(101) Why is the Delocalization Energy Negative and Why is it Proportional to the Number of Double Bonds? W. England and K. Ruedenberg, *J. Am. Chem. Soc.*, 95, 8769-8775 (1973).

(102) Even-Tempered Atomic Orbitals VI. Optimal Orbital Exponents and Optimal Orbital Contractions of Gaussian Primitives for Hydrogen, Carbon and Oxygen in Molecules, R. D. Bardo and K. Ruedenberg, *J. Chem. Phys.*, 60, 918-931 (1974).

(103) Even-Tempered Atomic Orbitals VII. Theoretical Equilibrium Geometries and Reaction Energies for Carbon Suboxide and Other Molecules Containing Carbon, Oxygen and Hydrogen, R. D. Bardo and K. Ruedenberg, *J. Chem. Phys.*, 60, 932-936 (1974).

(104) Genealogical Spin Eigenfunctions and Antisymmetric Many-Electron Wavefunctions Generated Directly from Young Diagrams, W. I. Salmon, *Advances in Quantum Chemistry* (P. O. Löwdin, Editor) Vol. 8, pp. 37-93 (Academic Press, 1974). Under supervision of K. Ruedenberg.

(105) Pictorial Representation of Three-Dimensional Distributions Through a Perspective View of Contour Diagrams in a Set of Parallel Planes, M. G. Dombek, J. J. Donn, K. R. Sundberg, K. Ruedenberg, USAEC Research and Development Report IS 3329, Ames Laboratory, USAEC, Iowa State University, 1974.

(106) Potential Energy Curve of the Cis-Trans-Isomerization of Glyoxal, K. R. Sundberg and L. M. Cheung, *Chem. Phys. Letters* 29, 93-97 (1974). Under supervision of K. Ruedenberg.

(107) Transferable Localized Molecular Orbitals for Acyclic Hydrocarbons, W. England, M. S.

Gordon and K. Ruedenberg, *Theor. Chim. Acta*, 37, 177-216 (1975).

(108) The Nature of the Chemical Bond, An Energetic View, K. Ruedenberg in "Localization and Delocalization in Quantum Chemistry" (R. Daudel, Editor) Vol. 1, 222-245 (D. Reidel Publ. Co., Dordrecht, Holland, 1975).

(109) MCSCF Studies of Chemical Reactions I. Natural Reaction Orbitals and Localized Reaction Orbitals, K. Ruedenberg and K. Sundberg in "Quantum Science" (J. L. Calais, O. Goscinski, J. Linderberg, Y. Öhrn, Eds.) pp. 505-515 (Plenum Publ. Co. N.Y. 1976).

(110) Approximate Relation between SCF Orbital Energies and Total SCF Energy, K. Ruedenberg, *J. Chem. Phys.*, 66, 375 (1977).

(111) Molecular Orbital Bonding Concepts in Polyatomic Molecules: A Novel Pictorial Approach, D. K. Hoffman, K. Ruedenberg, J. G. Verkade in *Structure and Bonding*, 33, 57-96 (1977).

(112) A Novel Pictorial Approach to Teach MO Bonding Concepts in Polyatomic Molecules, D. K. Hoffman, K. Ruedenberg, J. G. Verkade, *J. Chem. Ed.*, 54, 590-595 (1977).

(113) Beauty, Truth and Life, K. Ruedenberg, in "Changing Scene Highlights," Ames Laboratory, U.S. Department of Energy, Iowa State University, III, 53 (1977).

(114) Dimerization of Carbene to Ethylene, L. M. Cheung, K. R. Sundberg, K. Ruedenberg, *J. Am. Chem. Soc. (Communication)* 100, 8024 (1978).

(115) Determination of Orbitals and Selection of Configurations Through the Method of the Full Optimized Reaction Space, K. Ruedenberg in "Report on the NRCC 1978 Workshop on Post-Hartree-Fock Quantum Chemistry", pp. 46-64 (Lawrence Berkeley Laboratory, Univ. of California, Report LBL 8233, UC4, CONF 780883; 1979).

(116) MCSCF Optimization Through Combined Use of Natural Orbitals and the Brillouin-Levy-Berthier Theorem, K. Ruedenberg, L. M. Cheung, S. T. Elbert, *Int. J. Quantum Chemistry*, 16, 1069-1101 (1979).

(117) Electronic Rearrangements During Chemical Reactions II. Planar Dissociation of Ethylene, L. M. Cheung, K. R. Sundberg, K. Ruedenberg, *Intern. J. of Quantum Chemistry*, 16, 1103-1137 (1979).

(118) Systematic Approach to Extended Even-tempered Orbital Bases for Atomic and Molecular Calculations, D. F. Feller and K. Ruedenberg, *Theor. Chim. Acta*, 52, 231-251 (1979).

(119) Effective Convergence to Complete Orbital Bases and to the Atomic Hartree-Fock Limit through Systematic Sequences of Gaussian Primitives, M. W. Schmidt and K. Ruedenberg, *J. Chem. Phys.*, 71, 3951-3962 (1979).

- (120) MCSCF Optimization through Iterative CI Calculations in the Single Excitation Space and MCSCF Wave Functions in the Full Reaction Space, K. Ruedenberg, on pp. 51-57 of the "Proceedings of the NRCC Workshop on Recent Developments of Multiconfiguration Hartree-Fock Methods of July 15-17 at Texas A&M University". (Lawrence Berkeley Laboratory, Univ. of California, 1981).
- (121) The Sudden Polarization Effect: MCSCF Calculations on Planar and 90° Twisted Methylene cyclopropane, R. P. Johnson and M. W. Schmidt, *J. Am. Chem. Soc.* 103, 3244-3249 (1981). Under supervision of K. Ruedenberg.
- (122) Are Atoms Intrinsic to Molecular Wave Functions? I. The FORS Model, K. Ruedenberg, M. W. Schmidt, M. M. Gilbert, S. T. Elbert, *Chemical Physics*, 71, 41-49 (1982).
- (123) Are Atoms Intrinsic to Molecular Electronic Wave Functions? II. Analysis of FORS Orbitals, K. Ruedenberg, M. W. Schmidt, M. Gilbert, *Chemical Physics*, 71, 51-64 (1982).
- (124) Are Atoms Intrinsic to Molecular Electronic Wave Functions? III. Analysis of FORS Configurations, K. Ruedenberg, M. W. Schmidt, M. Gilbert, S. T. Elbert, *Chemical Physics*, 71, 65-78 (1982).
- (125) Concerted Dihydrogen Exchange between Ethane and Ethylene. SCF and FORS Calculations of the Barrier, D. F. Feller, M. W. Schmidt, K. Ruedenberg, *J. Am. Chem. Soc.* 104, 960-967 (1982).
- (126) Small Ring Cyclic Allenes: An ab-initio Study of the Structure of 1,2 Cyclohexadiene, M. W. Schmidt, R. O. Angus, R. P. Johnson, *J. Am. Chem. Soc.* 104, 6838 (1982). Under supervision of K. Ruedenberg.
- (127) Polarized Nonvertical Excited States: FORS MCSCF and CI Study of Torsion and Bending in Allene, B. Lam and R. P. Johnson, *J. Am. Chem. Soc.* 105, 7479 (1983). Under supervision of K. Ruedenberg.
- (128) Intra-Atomic Correlation Correction in the FORS Model, M. T. B. Lam, M. W. Schmidt, K. Ruedenberg, *J. Phys. Chem.*, 89, 2221-2235 (1985).
- (129) Chemical Binding and Electron Correlation in Diatomic Molecules as Described by the FORS Model and the FORS-IACC Model, M. W. Schmidt, M.T.B. Lam, S. T. Elbert, K. Ruedenberg, *Theor. Chim. Acta*, 68, 69-86 (1985).
- (130) Representation of Three-Dimensional Electron Distributions Through A Perspective View of Contour Diagrams in a Set of Parallel Planes, M. M. Gilbert, J. J. Donn, M. Peirce, K. R. Sundberg, K. Ruedenberg, *J. Computational Chemistry*, 6, 209-215 (1985).
- (131) Electron Difference Densities and Chemical Binding, P. Valtazanos, W. H. E. Schwarz and K. Ruedenberg, *Theoretica Chimica Acta*, 68, 471-506 (1985).

- (132) Small Ring Cyclic Cumulenes: Theoretical Studies of the Structure and Barrier to Inversion in Cyclic Allenes, R. O. Angus, M. W. Schmidt, R. P. Johnson, *J. Am. Chem. Soc.* 107, 532-537 (1985). Under supervision of K. Ruedenberg.
- (133) A Chemically Useful Definition of Electron Difference Densities, W. H. E. Schwarz, L. Mensching, P. Valtazanos, W. von Niessen, *Int. J. Quantum Chem.*, 29, 909-914 (1986). Under supervision of K. Ruedenberg.
- (134) Gradient Extremals, D. K. Hoffman, R. S. Nord, K. Ruedenberg. *Theor. Chim. Acta*, 69, 265-279 (1986).
- (135) Bifurcations and Transition States, P. Valtazanos and K. Ruedenberg, *Theoretica Chimica Acta*, 69, 281-307 (1986).
- (136) Ring Opening of Cyclopropylidenes to Allenes: Reactions with Bifurcating Transition Regions, Free Internal Motions, Steric Hindrances and Long-Range Dipolar Interactions, P. Valtazanos, S. T. Elbert, K. Ruedenberg, *J. Am. Chem. Soc.*, 108, 3147-3148 (1986) (Comm. to the Editor).
- (137) Generation of a Full Active Configuration Space in Terms of Symmetry- and Spin-Adapted Antisymmetrized Orbital Products, M. T. B. Lam, S. T. Elbert and K. Ruedenberg, *Intern. J. Quantum Chem.* 31, 489-505 (1987).
- (138) X-Ray Diffraction, Electron Densities and Chemical Bonding, W. H. E. Schwarz, L. Mensching, K. Ruedenberg, R. Jacobson, L. L. Miller, Portugal, *Phys.* 19, 185-189 (1988).
- (139) International Evaluation of Theoretical Chemistry in Sweden, A. D. Buckingham, R. Manne, J. S. Rowlinson, K. Ruedenberg, A. Warshel, B. Nordén; Swedish Natural Science Research Council, 1988.
- (140) Chemical Deformation Densities. I. Formulation and Quantitative Determination, W. H. E. Schwarz, K. Ruedenberg, L. Mensching, *J. Am. Chem. Soc.*, 111, 6926-6933 (1989).
- (141) Chemical Deformation Densities. II. Small Molecules, L. Mensching, W. von Niessen, P. Valtazanos, K. Ruedenberg, W. H. E. Schwarz, *J. Am. Chem. Soc.*, 111, 6933-6941 (1989).
- (142) Electron Densities, Deformation Densities, and Chemical Bonding, W. H. E. Schwarz, L. Mensching, K. Ruedenberg, L. L. Miller, P. Valtazanos, W. von Niessen, R. A. Jacobson, *Angew. Chem.* 101, 605 (1989) and *Intl. Ed.* 28, 597-600 (1989).
- (143) Nonspherical Atom Densities and Chemical Deformation Densities from X-Ray Scattering, K. Ruedenberg and W. H. E. Schwarz, *J. Chem. Phys.*, 92, 4956-4969 (1990).
- (144) The Potential Energy Surface of the Ground State of Carbon Dioxide, S. S. Xantheas, S. T. Elbert and K. Ruedenberg, *Chem. Phys. Letters*, 166, 39-42 (1990).

- (145) An Intersection Seam between the Ground State of Ozone and an Excited State of Like Symmetry, K. Ruedenberg, S. Xantheas, S. T. Elbert, *J. Chem. Phys.*, 93, 7519-7521 (1990).
- (146) The Ring Opening of Cyclopropylidene to Allene: Global Features of the Reaction Surface, P. Valtazanos, S. T. Elbert, S. Xantheas, K. Ruedenberg, *Theor. Chim. Acta*, 78, 287-326 (1991).
- (147) The Ring Opening of Cyclopropylidene to Allene and the Isomerization of Allene: Ab-Initio Interpretation of the Electronic Rearrangements in terms of Quasiatomic Orbitals, S. Xantheas, P. Valtazanos, K. Ruedenberg, *Theor. Chim. Acta*, 78, 327-364 (1991).
- (148) The Ring Opening of Cyclopropylidene to Allene: Key Features of the Accurate Reaction Surface. P. Valtazanos, S. Xantheas, S. T. Elbert, K. Ruedenberg, *Theor. Chim. Acta*, 78, 365-396 (1991).
- (149) The Ring Opening of Substituted Cyclopropylidene to Substituted Allene: The Effect of Steric and Long-Range Electrostatic Interactions, P. Valtazanos and K. Ruedenberg, *Theor. Chim. Acta*, 78, 397-416 (1991).
- (150) Potential Energy Surfaces of Ozone. I, S. S. Xantheas, G. J. Atchity, S. T. Elbert, K. Ruedenberg, *J. Chem. Phys.*, 94, 8054-8069 (1991).
- (151) Potential Energy Surfaces Near Intersections, G. J. Atchity, S. S. Xantheas, K. Ruedenberg, *J. Chem. Phys.*, 95, 1862-1876 (1991).
- (152) Efficient Use of Jacobi Rotations for Orbital Optimization and Localization, R. C. Raffenetti, K. Ruedenberg, C. L. Janssen, H. F. Schaefer, *Theor. Chim. Acta*, 86, 149-165 (1993).
- (153) Gradient Extremals and Steepest Descent Lines on Potential Energy Surfaces, J. Q. Sun and K. Ruedenberg, *J. Chem. Phys.*, 98, 9707-9714 (1993).
- (154) Strong Shifts in Diabatic Nondynamic Correlations Cause Conical Intersection between Low-Lying Closed-Shell Adiabatic Singlets of Like Symmetry in Ozone, G. J. Atchity and K. Ruedenberg. *J. Chem. Phys.*, 99, 3790-3798 (1993).
- (155) A Quantum Chemical Determination of Diabatic States, K. Ruedenberg and G. J. Atchity. *J. Chem. Phys.* 99, 3799-3803 (1993).
- (156) Quadratic Steepest Descent on Potential Energy Surfaces. I. Basic Formalism and Quantitative Assessment, J. Q. Sun and K. Ruedenberg. *J. Chem. Phys.* 99, 5257-5268 (1993).
- (157) Quadratic Steepest Descent on Potential Energy Surfaces. II. Reaction Path Following without Analytic Hessians, J. Q. Sun and K. Ruedenberg. *J. Chem. Phys.* 99, 5269-5275 (1993).
- (158) Quadratic Steepest Descent on Potential Energy Surfaces. III. Minima Seeking along

- Steepest Descent Lines, J. Q. Sun and K. Ruedenberg. *J. Chem. Phys.* 99, 5276-5280 (1993).
- (159) Historical Notes on Doctor Faustus, K. Ruedenberg, *The Puppetry Journal of the Puppeteers of America*, 44, 8 (1993).
- (160) Potential Energy Surfaces of Carbon Dioxide, S. S. Xantheas and K. Ruedenberg. *Intern. J. Quantum Chem.*, 49, 409-427 (1994).
- (161) Gradient Fields of Potential Energy Surfaces, K. Ruedenberg and J. Q. Sun. *J. Chem. Phys.* 100, 5836-5848 (1994).
- (162) Quadratic Descent on Potential Energy Surfaces. IV. Adaptation to Singular Hessians, K. Ruedenberg and J. Q. Sun. *J. Chem. Phys.* 100, 6101 (1994).
- (163) Locating Transition States by Quadratic Image Gradient Descent on Potential Energy Surfaces, J. Q. Sun and K. Ruedenberg. *J. Chem. Phys.* 101, 2157-2167 (1994).
- (164) A Simple Prediction of Approximate Transition States on Potential Energy Surfaces, K. Ruedenberg and J. Q. Sun. *J. Chem. Phys.* 101, 2168-2174 (1994).
- (165) Rotation Matrices for Real Spherical Harmonics. Direct Determination by Recursion, J. Ivanic and K. Ruedenberg, *J. Phys. Chem.* 100, 6342-6347 (1996).
- (166) Global Potential Energy Surfaces of the Lowest Two $^1A'$ States of Ozone, G. J. Atchity and K. Ruedenberg. *Theor. Chem. Acc.* 96, 176-194 (1997).
- (167) The Global Intersection Seam between the Lowest Two $^1A'$ States of Ozone, G. J. Atchity, K. Ruedenberg, A. Nanayakkara. *Theor. Chem. Acc.* 96, 195-204 (1997).
- (168) Perimetric Scale-Shape Coordinates for Triatomic Molecules. G. J. Atchity and K. Ruedenberg, *Theor. Chem. Acc.* 96, 205-211 (1997).
- (169) Electron Densities on pp-AO Occupancies in p-Bonded Systems, J. E. Niu, W. H. E. Schwarz, K. Ruedenberg, *J. Mol. Struct. (Theochem)* 389, 117-128 (1997)
- (170) Determination of Diabatic States Through Enforcement of Configurational Uniformity, K. Ruedenberg and G. J. Atchity. *Theor. Chem. Acc.* 97, 47-58 (1997)
- (171) Violation of the Weak Non-Crossing Rule between Totally Symmetric Closed Shell States in the Valence-Isoelectronic Series O_3 , S_3 , SO_2 , S_2O , G. J. Atchity, J. Ivanic, K. Ruedenberg, *J. Chem. Phys.*, 107, 4307-4317 (1997).
- (172) Robert S. Hansen, An Eulogy at the first R. S. Hansen Lecture, K. Ruedenberg, Golden Alumni, Chemistry Department, Iowa State University, March 1999.
- (173) A Local Understanding of the Quantum Chemical Geometric Phase Theorem for Potential

Energy Surface Intersections, G.J. Atchity, K. Ruedenberg, J.Chem.Phys, 110, 4208-4221(1999)

(174) Orbital Transformations and Configurational Transformations of Electronic Wave Functions, G. J. Atchity and Klaus Ruedenberg, J. Chem. Phys., 111, 2910-2920 (1999)

(175) Rapid and Stable Determination of Rotation Matrices between Spherical Harmonics by Direct Recursion, Cheol Ho Choi, Joseph Ivanic, Mark S. Gordon, Klaus Ruedenberg, J. Chem. Phys., 111, 8825-8831 (1999)

(176) A New Parallel Optimal-Parameter Fast Multipole Method, Cheol Ho Choi, Klaus Ruedenberg, Mark S. Gordon, J. Computational Chem., 22, 1484-1501 (2001)

(177) Oriented Non-spherical Atoms in Crystals Deduced from X-Ray Scattering Data, L. L. Miller, R. A. Jacobson, K. Ruedenberg, J. Niu, W. H. E. Schwarz, Helvetica Chimica Acta, 84, 1907-1942 (2001)

(178) Identification of Deadwood in Configuration Spaces through General Direct Configuration Interaction. Joseph Ivanic and Klaus Ruedenberg, Theor. Chem. Accounts, 106, 339-351 (2001)

(179) Deadwood in Configuration Spaces. II. SD and SDTQ Spaces, Joseph Ivanic and Klaus Ruedenberg, Theor. Chem. Accounts, 107, 220-228 (2002)

(180) Electron Pairs, Localized Orbitals and Electron Correlation, Laimutis Bytautas and Klaus Ruedenberg, Molecular Physics, 100, 757-781 (2002)

(181) A MCSCF Method for Ground and Excited States Based on Full Optimizations of Successive Jacobi Rotations, Joseph Ivanic and Klaus Ruedenberg, J. Computational Chemistry 24, 1250-1262 (2003)

(182) Split-Localized Orbitals Can Yield Stronger Configuration Interaction Convergence than Natural Orbitals, L. Bytautas, J. Ivanic, K. Ruedenberg, J. Chem. Phys. 119, 8217 (2003)

(183) Molecule Intrinsic Minimal Basis Sets. I. Exact Resolution of Ab-Initio Optimized Molecular Orbitals in terms of Deformed Atomic Minimal-Basis Orbitals, W. C. Lu, C. Z. Wang, M. W. Schmidt, L. Bytautas, K. M. Ho, K. Ruedenberg, J. Chem. Phys. 120, 2629-2637 (2004)

(184) Molecule Intrinsic Minimal Basis Sets. II. Bonding Analyses for Si_4H_6 and Si_2 to Si_{10} , W. C. Lu, C. Z. Wang, M. W. Schmidt, L. Bytautas, K. M. Ho, K. Ruedenberg, J. Chem. Phys. 120, 2638-2651 (2004)

(185) Exact Representation of Electronic Structures in Crystals in Terms of Highly Localized Quasiatomic Minimal Basis Orbitals, W. C. Lu, C. Z. Wang, T. L. Chan, K. Ruedenberg, and K. M. Ho, Phys. Rev. B, 70, 04110(R) (2004)

- (186) Correlation Energy Extrapolation Through Intrinsic Scaling. I. Laimutis Bytautas and Klaus Ruedenberg, *J. Chem. Phys.*, 121, 10905 (2004)
- (187) Correlation Energy Extrapolation Through Intrinsic Scaling. II. Laimutis Bytautas and Klaus Ruedenberg, *J. Chem. Phys.*, 121, 10919 (2004)
- (188) Correlation Energy Extrapolation Through Intrinsic Scaling. III. Compact Wavefunctions. Laimutis Bytautas and Klaus Ruedenberg, *J. Chem. Phys.*, 121, 10852 (2004)
- (189) Correlation Energy Extrapolation Through Intrinsic Scaling. IV. Accurate Binding Energies of the Homonuclear Diatomic Molecules Carbon, Nitrogen, Oxygen and Fluorine. Laimutis Bytautas and Klaus Ruedenberg, *J. Chem. Phys.*, 122, 154110 (2005)
- (190) Transferability of the Slater-Koster Tight-Binding Scheme from a First-Principles Perspective. W. C. Lu, C. Z. Wang, K. Ruedenberg and K. M. Ho, *Phys. Rev. B* 72, 205123 (2005)
- (191) Correlation Energy Extrapolation Through Intrinsic Scaling. V. Electronic Energy, Atomization Energy and Enthalpy of Formation of Water, L. Bytautas and K. Ruedenberg. *J. Chem. Phys.*, 124, 174304 (2006)
- (192) Scalable Correlated Electronic Structure Theory. Mark S. Gordon, Klaus Ruedenberg, Michael W. Schmidt, Laimis Bytautas, Timothy J. Dudley, Takeshi Nagata, Ryan Olson, Sergey Varganov, *J. of Physics: Conference Series* 46, 229-233 (2006).
- (193) Why Does Electron Sharing Lead to Covalent Bonding? A Variational Analysis. Klaus Ruedenberg and Michael W. Schmidt. *J. Comp. Chem.*, 28, 391-410 (2007).
- (194) Toward a Physical Understanding of Electron-Sharing Two-Center Bonds. I. General Aspects. T. Bitter, K. Ruedenberg, W.H.E. Schwarz, *J. Comp. Chem.*, 28, 411-422 (2007).
- (195) Economical Description of Electron Correlation, L. Bytautas and K. Ruedenberg, in *Advances in Electron Correlation Methodology* (A. K. Wilson and K. A. Peterson Edtrs), ACS Symposium Series Volume 958, p. 103-123 (2007).
- (196) Accurate *Ab Initio* Potential Energy Curve of F₂. I. Non-Relativistic Full Valence CI Energies by the CEEIS Method. L. Bytautas, T. Nagata, M. S. Gordon, K. Ruedenberg, *J. Chem. Phys.* 127, 164317, 1-18 (2007).
- (197) Accurate *Ab Initio* Potential Energy Curve of F₂. II. Core-Valence Correlations, Relativistic Contributions and Long-Range Interactions. L. Bytautas, N. Matsunaga, T. Nagata, M. S. Gordon, K. Ruedenberg, *J. Chem. Phys.* 127, 204301, 1-12 (2007).
- (198) Accurate *Ab Initio* Potential Energy Curve of F₂. III. The Vibration Rotation Spectrum. L. Bytautas, N. Matsunaga, T. Nagata, M. S. Gordon, K. Ruedenberg, *J. Chem. Phys.* 127, 204313, 1-20 (2007).

- (199) Correlation Energy and Dispersion Interaction in the *ab initio* Potential Energy Curve of the Neon Dimer. L. Bytautas and K. Ruedenberg, *J. Chem. Phys.*, 128, 214308, 1-12 (2008).
- (200) 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. J. Ivanic, G. J. Atchity and K. Ruedenberg, *Theor. Chem. Acc.*, 120, 281-294 (2008).
- (201) 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→NOH. J. Ivanic and K. Ruedenberg, *Theor. Chem. Acc.*, 120, 295-305 (2008).
- (202) *A-Priori* Identification of Configurational Deadwood. Laimutis Bytautas and Klaus Ruedenberg, *Chem. Phys.*, 356, 64-75 (2009)
- (203) *Ab Initio* Potential Energy curve of F₂. IV. Transition from the covalent to the van der Waals region. Competition between multipolar and correlation forces. L. Bytautas and K. Ruedenberg, *J. Chem. Phys.* 130, 204101, 1-14 (2009)
- (204) Physical Understanding through Variational Reasoning: Electron Sharing and Covalent Bonding. K. Ruedenberg and M.W. Schmidt, *J. Phys. Chem.*, 113, 1954-1968 (2009)
- (205) Accurate *ab initio* potential energy curve of O₂. I. Non-relativistic full CI valence correlation by the CEEIS method. L. Bytautas and K. Ruedenberg, *J. Chem. Phys.* 132, 074109, 1-10 (2010)
- (206) Accurate *ab initio* potential energy curve of O₂. II. Core-valence correlations, relativistic contributions and vibration-rotation spectrum. L. Bytautas, N. Matsunaga, K. Ruedenberg, *J. Chem. Phys.* 132, 074307, 1-15 (2010)
- (207) Autobiography. K. Ruedenberg, *J. Phys. Chem. A* 114, 8490–8495 (2010)
- (208) The range of electron correlation between localized molecular orbitals. A full configuration interaction analysis for the NCCN molecule. L. Bytautas and K. Ruedenberg, *J. Phys. Chem. A* 114, 8601–8612 (2010)
- (209) Electronic structure analysis of the ground state potential energy curve of Be₂. M.W. Schmidt, J. Ivanic, K. Ruedenberg, *J. Phys. Chem. A* 114, 8687-8696 (2010)
- (210) Analysis of the bonding patterns in the valence isoelectronic series O₃, S₃, SO₂ and OS₂ in terms of oriented quasi-atomic molecular orbitals. V.A. Glezakou, S.T. Elbert, S. S. Xantheas, K. Ruedenberg, *J. Phys. Chem. A* 114, 8923–8931 (2010)

- (211) Toward a Physical Understanding of Electron-Sharing Two-Center Bonds. II. A Pseudo-Potential Based Approach. T. Bitter, S.G. Wang, K. Ruedenberg, W.H.E. Schwarz, *Theor Chem Acc.* 127, 237–257 (2010)
- (212) Accurate potential energy curve for B₂. *Ab initio* elucidation of the experimentally elusive ground state rotation-vibration spectrum. L. Bytautas, N.Matsunaga, G. Scuseria, K. Ruedenberg, *J. Phy. Chem. A.*, 116, 1717-1729 (2012)
- (213) The dispersion interaction between quantum mechanics and effective fragment potential molecules. Q.A. Smith, K. Ruedenberg, M.S. Gordon, L.V. Slipchenko, *J. Chem. Phys.* 136, 244107 (2012)
- (214) Three Millennia of Atoms and Molecules. K. Ruedenberg and W.H.E. Schwarz, Chapter 1 in the book "Pioneers of Quantum Chemistry" (T. Strom and A. Wilson Editors, American Chemical Society, ACS Symposium Series 1122, 2013) pp. 1 - 45
- (215) Unusual Inorganic Biradicals: A Theoretical Analysis. E. Miliordos, K. Ruedenberg, S. S. Xantheas, *Angewandte Chemie, International Edition* 52, (Issue 22) 5736–5739 (2013)
- (216) A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions. A. C. West, M. W. Schmidt, M. S. Gordon, and K. Ruedenberg, *J. Chem. Phys.* 139, 234107, 18 pages (2013)
- (217) Accurate *ab initio* potential energy curves and spectroscopic properties of the four lowest singlet states of C₂. J. S. Boschen, D. Theis, K. Ruedenberg, T.L. Windus, *Theor Chem Acc* 133, 1425, 12 pages (2014)
- (218) Covalent bonds are created by the drive of electron waves to lower their kinetic energy through expansion. M. W. Schmidt, J. Ivanic, K. Ruedenberg, *J. Chem. Phys.* 140, 204104, 14 pages (2014)
- (219) The Physical Origin of Covalent Binding. M. W. Schmidt, J. Ivanic, K. Ruedenberg, Chapter 1, pp. 1-67 of the book "The Chemical Bond. Fundamental Aspects of Chemical Bonding," (Edited by G. Frenking and S. Shaik, Wiley-VCH, 2014)
- (220) Weighted orthogonalization of atomic orbitals: A stable alternative to the Carlson–Keller method, Aaron C. West, *Comp. and Theor. Chem.* 1045, 73–77 (2014) (under supervision of K. Ruedenberg)
- (221) In Memoriam Hermann Hartmann, founder of TCA, on the occasion of his 100th Birthday. W. H. Eugen Schwarz, Fritz Grein, Klaus Ruedenberg, *Theor Chem Acc*, 133, 1508, 2 pages (2014)
- (222) Six Question on Topology in Theoretical Chemistry. Paul Ayers, Russell Boyd, Patrick Bultinck, Michel Caffarel, Ramon Carbó-Dorca, Mauro Causáf, Jerzy Cioslowski, Julia Contreras-Garcia, David L. Cooper, Philip Coppens, Carlo Gatti, Simon Grabowsky, Paolo

Lazzeretti, Ángel Martín, Pendás, Paul Popelier, Klaus Ruedenberg, Henry Rzepa, Andreas Savin, Alexander Sax, W. H. Eugen Schwarz, Shant Shahbazian, Bernard Silvi, Miquel Solà, Vladimir Tsirelson, *Computational and Theoretical Chemistry* 1053, 2–16 (2015)

(223) Seniority number description of potential energy surfaces: Symmetric dissociation of water, N₂, C₂, and Be₂. Laimutis Bytautas, Gustavo E. Scuseria, Klaus Ruedenberg, *J. Chem. Phys.* 143, 094105, 15 pages (2015)

(224) A comprehensive analysis in terms of molecule-intrinsic, quasi-atomic orbitals. II. Strongly correlated wave functions. Aaron C. West, Michael W. Schmidt, Mark S. Gordon, Klaus Ruedenberg, *J. Phys. Chem. A* 119, 10360–10367 (2015), DOI: 10.1021/acs.jpca.5b03399

(225) A comprehensive analysis in terms of molecule-intrinsic, quasi-atomic orbitals. III. The covalent bonding structure of urea. Aaron C. West, Michael W. Schmidt, Mark S. Gordon, Klaus Ruedenberg, *J. Phys. Chem. A* 119, 10368–10375 (2015), DOI: 10.1021/acs.jpca.5b03400

(226) A comprehensive analysis in terms of molecule-intrinsic quasi-atomic orbitals. IV. Bond breaking and bond forming along the dissociative reaction path of dioxetane. Aaron C. West, Michael W. Schmidt, Mark S. Gordon, Klaus Ruedenberg, *J. Phys. Chem. A* 119, 10376–10389 (2015), DOI: 10.1021/acs.jpca.5b03402

(227) 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. Daniel Theis, Joseph Ivanic, Theresa L. Windus, Klaus Ruedenberg, *J. Chem. Phys.* 144, 104304 (2016), 18 pages, DOI: 10.1063/1.4942019

(228) Correlation Energy Extrapolation by Many-Body Expansion. Jeffery S. Boschen, Daniel Theis, Klaus Ruedenberg, Theresa L. Windus. *J. Phys. Chem. A*, 121, 836–844, (2017) DOI: 10.1021/acs.jpca.6b10953

(229) Intrinsic resolution of molecular electronic wave functions and energies in terms of quasi-atoms and their interactions. Aaron C. West, Michael W. Schmidt, Mark S. Gordon, Klaus Ruedenberg, *J. Phys. Chem. A*, 121, 1086–1105 (2017) DOI: 10.1021/acs.jpca.6b10911

(230) Relativistic *ab initio* accurate minimal basis sets: Quantitative LUMOs and oriented quasi-atomic orbitals for the elements Li – Xe. George Schoendorff; Aaron C. West.; Michael W. Schmidt; Klaus Ruedenberg; Angela Wilson; Mark Gordon, *J. Phys. Chem. A*, 121, 3588–3597 (2017), DOI: 10.1021/acs.jpca.7b01916

(231) Identification and characterization of molecular bonding structures by *ab initio* quasi-atomic orbital analyses. Aaron C. West, Juan J. Duchimaza-Heredia, Mark S. Gordon, Klaus Ruedenberg. *J. Phys. Chem. A* (2017), 121, 8884–8898 DOI: 10.1021/acs.jpca.7b07054 .

(232) Atom-Based Strong Correlation Method: An Orbital Selection Algorithm. Aaron C. West. *J. Phys. Chem. A*, **2017**, *121*, 8912–8926. DOI: 10.1021/acs.jpca.7b08482 (under supervision of K.Ruedenberg)

(233) Dispersion Interactions in QM/EFP. Lyudmila Slipchenko, Mark Gordon, Klaus Ruedenberg, *J. Phys. Chem. A* (**2017**), *121*, 9495–9507. DOI: 10.1021/acs.jpca.7b05875

(234) Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. Juan J. Duchimaza Heredia, Klaus Ruedenberg, Mark S. Gordon, *J. Phys. Chem. A* (**2018**), *122*, 3442–3454. DOI: 10.1021/acs.jpca.8b00115

(235) The Virial Theorem and Covalent Binding. George B. Bacskay, Sture Nordholm and Klaus Ruedenberg, *J. Phys. Chem. A* (**2018**) *122*, 7880-7893. DOI: 10.1021/acs.jpca.8b08234

(236) *Quasi-atomic bond analyses in the sixth period. I. Relativistic accurate atomic minimal basis sets for the elements cesium to radon.* George S. Schoendorff, Aaron C. West, Michael W. Schmidt, Klaus Ruedenberg, Mark S. Gordon, *J. Phys. Chem. A*, (**2019**) *123*, 5242–5248. DOI: 10.1021/acs.jpca.9b04023

(237) *Quasi-atomic bond analyses in the sixth period. II. Bond analyses of cerium oxides.* George S. Schoendorff, Michael W. Schmidt, Klaus Ruedenberg, Mark S. Gordon, *J. Phys. Chem. A*, (**2019**) *123*, 5249–5256. DOI: 10.1021/acs.jpca.9b04024

(238) Giuseppe M. J. Barca, Colleen Bertoni, Laura Carrington, Dipayan Datta, Nuwan DeSilva, J. Emiliano Deustua, Dmitri G. Fedorov, Jeffrey R. Gour, Anastasia O. Gunina, Emilie Guidez, Taylor Harville, Stephan Irle, Joe Ivanic, Karol Kowalski, Sarom S. Leang, Hui Li, Wei Li, Jesse J. Lutz, Ilias Magoulas, Joani Mato, Vladimir Mironov, Hiroya Nakata, Buu Q. Pham, Piotr Piecuch, David Poole, Spencer R. Pruitt, Alistair P. Rendell, Luke B. Roskop, Klaus Ruedenberg, Tosaporn Sattasathuchana, Michael W. Schmidt, Jun Shen, Lyudmila Slipchenko, Masha Sosonkina, Vaibhav Sundriyal, Ananta Tiwari, Jorge L. Galvez Vallejo, Bryce Westheimer, Marta Włoch, Peng Xu, Federico Zahariev, and Mark S. Gordon: “Recent Developments in the General Atomic and Molecular Electronic Structure System”, *J. Chem. Phys.*, (**2020**) *152*, 154201.

(239) *Why is Si₂H₂ not linear? An intrinsic quasi-atomic bonding analysis.* Emilie B. Guidez, Mark S. Gordon, Klaus Ruedenberg, *J. Am. Chem. Soc.* (**2020**), *142*, 13729–13742. dx.doi.org/10.1021/jacs.0c03082

(240) *Multiple bonding in rhodium monoboride. Quasi-atomic analyses of the ground and low-lying excited states.* George Schoendorff, Klaus Ruedenberg, and Mark S. Gordon, *J. Phys. Chem. A*, (**2021**) *125*, 4836–4846. doi.org/10.1021/acs.jpca.1c02860

(241) *Atoms and interatomic bonding synergism inherent in molecular electronic wave functions*, Klaus Ruedenberg, *J. Chem. Phys.* (**202?**) Submitted

