

Martin Kaupp

List of Publications by Year in descending order

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10970
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| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107. | 1.2 | 616 |
| 2 | Pseudopotential approaches to Ca, Sr, and Ba hydrides. Why are some alkaline earth MX ₂ compounds bent?. <i>Journal of Chemical Physics</i> , 1991, 94, 1360-1366. | 1.2 | 562 |
| 3 | How Do Spin-Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin-Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. <i>Chemistry - A European Journal</i> , 1998, 4, 118-126. | 1.7 | 344 |
| 4 | Exciton Trapping in π -Conjugated Materials: A Quantum-Chemistry-Based Protocol Applied to Perylene Bisimide Dye Aggregates. <i>Journal of the American Chemical Society</i> , 2008, 130, 12858-12859. | 6.6 | 290 |
| 5 | The DFT route to NMR chemical shifts. <i>Journal of Computational Chemistry</i> , 1999, 20, 91-105. | 1.5 | 274 |
| 6 | A Critical Validation of Density Functional and Coupled-Cluster Approaches for the Calculation of EPR Hyperfine Coupling Constants in Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9966-9983. | 1.1 | 271 |
| 7 | From Bis(silylene) and Bis(germylene) Pincer-Type Nickel(II) Complexes to Isolable Intermediates of the Nickel-Catalyzed Sonogashira Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 15617-15626. | 6.6 | 232 |
| 8 | Density Functional Calculations of Electronic g-Tensors Using Spin-Orbit Pseudopotentials and Mean-Field All-Electron Spin-Orbit Operators. <i>Journal of the American Chemical Society</i> , 2000, 122, 9206-9218. | 6.6 | 222 |
| 9 | A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Dirac-Kohn-Sham equation. <i>Journal of Chemical Physics</i> , 2008, 128, 104101. | 1.2 | 196 |
| 10 | A Reliable Quantum-Chemical Protocol for the Characterization of Organic Mixed-Valence Compounds. <i>Journal of the American Chemical Society</i> , 2009, 131, 16292-16302. | 6.6 | 184 |
| 11 | The highest oxidation states of the transition metal elements. <i>Coordination Chemistry Reviews</i> , 2009, 253, 606-624. | 9.5 | 183 |
| 12 | Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. <i>Journal of Computational Chemistry</i> , 2002, 23, 794-803. | 1.5 | 182 |
| 13 | The question of bending of the alkaline earth dihalides MX ₂ (M = beryllium, magnesium, calcium,). <i>Journal of the American Chemical Society</i> , 1991, 113, 6012-6020. | 6.6 | 180 |
| 14 | Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. <i>Chemical Society Reviews</i> , 2014, 43, 5067-5088. | 18.7 | 168 |
| 15 | Where Is the Spin? Understanding Electronic Structure and g-Tensors for Ruthenium Complexes with Redox-Active Quinonoid Ligands. <i>Journal of the American Chemical Society</i> , 2005, 127, 11399-11413. | 6.6 | 164 |
| 16 | Non-VSEPR Structures and Bonding in d ⁰ Systems. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 3534. | 7.2 | 158 |
| 17 | Mechanisms of EPR Hyperfine Coupling in Transition Metal Complexes. <i>Journal of the American Chemical Society</i> , 2000, 122, 11900-11913. | 6.6 | 148 |
| 18 | From silicon(II)-based dioxygen activation to adducts of elusive dioxasiliranes and sila-ureas stable at room temperature. <i>Nature Chemistry</i> , 2010, 2, 577-580. | 6.6 | 140 |

| # | ARTICLE | IF | CITATIONS |
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| 19 | Ab initio study of structures and stabilities of substituted lead compounds. Why is inorganic lead chemistry dominated by PbII but organolead chemistry by PbIV?. Journal of the American Chemical Society, 1993, 115, 1061-1073. | 6.6 | 132 |
| 20 | Carboalumination of a chromium–chromium quintuple bond. Nature Chemistry, 2009, 1, 322-325. | 6.6 | 131 |
| 21 | Mercury Is a Transition Metal: The First Experimental Evidence for HgF ₄ . Angewandte Chemie - International Edition, 2007, 46, 8371-8375. | 7.2 | 126 |
| 22 | ¹³ C NMR Study of Halogen Bonding of Haloarenes: Measurements of Solvent Effects and Theoretical Analysis. Journal of the American Chemical Society, 2004, 126, 4412-4419. | 6.6 | 121 |
| 23 | Computational and spectroscopic studies of organic mixed-valence compounds: where is the charge?. Physical Chemistry Chemical Physics, 2011, 13, 16973. | 1.3 | 121 |
| 24 | Relativistic Four-Component DFT Calculations of ¹ H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckingham–Stephens Model. Journal of Physical Chemistry A, 2011, 115, 5654-5659. | 1.1 | 120 |
| 25 | The role of radial nodes of atomic orbitals for chemical bonding and the periodic table. Journal of Computational Chemistry, 2007, 28, 320-325. | 1.5 | 119 |
| 26 | Theoretical and experimental study of diamagnetic and paramagnetic products from thermal and light-induced alkyl transfer between zinc or magnesium dialkyls and 1,4-diaza-1,3-butadiene substrates. Journal of the American Chemical Society, 1991, 113, 5606-5618. | 6.6 | 118 |
| 27 | Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. Journal of Chemical Physics, 2016, 144, 074106. | 1.2 | 117 |
| 28 | A thermochemically competitive local hybrid functional without gradient corrections. Journal of Chemical Physics, 2007, 126, 011103. | 1.2 | 113 |
| 29 | Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. Chemical Reviews, 2020, 120, 7065-7103. | 23.0 | 113 |
| 30 | Spin-orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms?. Chemical Physics Letters, 1998, 296, 93-104. | 1.2 | 112 |
| 31 | The structural variations of monomeric alkaline earth MX ₂ compounds (M = calcium, strontium, barium). Journal of the American Chemical Society, 1992, 114, 491-497. | 6.6 | 108 |
| 32 | A Neutral, Monomeric Germanium(I) Radical. Journal of the American Chemical Society, 2011, 133, 10074-10077. | 6.6 | 108 |
| 33 | The equilibrium structures of monomeric Group 2 and lanthanide(II) metallocenes MCp ₂ (M = calcium, strontium, barium). Journal of the American Chemical Society, 1992, 114, 8202-8208. | 6.6 | 107 |
| 34 | Metal–Metal Distances at the Limit: Cr–Cr 1.73 Å... the Importance of the Ligand and its Fine Tuning. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1149-1152. | 0.6 | 107 |
| 35 | Combining NMR spectroscopy and quantum chemistry as tools to quantify spin density distributions in molecular magnetic compounds. Coordination Chemistry Reviews, 2009, 253, 2376-2386. | 9.5 | 106 |
| 36 | Activation of Ammonia by a Si=O Double Bond and Formation of a Unique Pair of Sila-Hemiaminal and Silanoic Amide Tautomers. Journal of the American Chemical Society, 2010, 132, 6912-6913. | 6.6 | 106 |

| # | ARTICLE | IF | CITATIONS |
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| 37 | Understanding Ground- and Excited-State Properties of Perylene Tetracarboxylic Acid Bisimide Crystals by Means of Quantum Chemical Computations. <i>Journal of the American Chemical Society</i> , 2009, 131, 15660-15668. | 6.6 | 104 |
| 38 | Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit pseudopotentials. <i>Journal of Chemical Physics</i> , 2001, 114, 61. | 1.2 | 101 |
| 39 | Impact of Molecular Flexibility on Binding Strength and Self-Sorting of Chiral π -Surfaces. <i>Journal of the American Chemical Society</i> , 2011, 133, 9580-9591. | 6.6 | 101 |
| 40 | Breakdown of Bond Length-Bond Strength Correlation: A Case Study. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4607-4609. | 7.2 | 100 |
| 41 | Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. <i>Coordination Chemistry Reviews</i> , 2017, 344, 355-362. | 9.5 | 99 |
| 42 | Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. <i>Journal of Chemical Physics</i> , 2007, 126, 024107. | 1.2 | 98 |
| 43 | Local hybrid exchange-correlation functionals based on the dimensionless density gradient. <i>Chemical Physics Letters</i> , 2007, 440, 160-168. | 1.2 | 98 |
| 44 | Interpretation of ^{13}C NMR chemical shifts in halomethyl cations. On the importance of spin-orbit coupling and electron correlation. <i>Chemical Physics Letters</i> , 1997, 265, 55-59. | 1.2 | 95 |
| 45 | Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1378. | 6.2 | 95 |
| 46 | Density Functional Calculations of Electronic g -Tensors for Semiquinone Radical Anions. The Role of Hydrogen Bonding and Substituent Effects. <i>Journal of the American Chemical Society</i> , 2002, 124, 2709-2722. | 6.6 | 94 |
| 47 | Insight into the Mechanism of Carbonyl Hydrosilylation Catalyzed by Brookhart's Cationic Iridium(III) Pincer Complex. <i>Journal of the American Chemical Society</i> , 2014, 136, 6912-6915. | 6.6 | 93 |
| 48 | Dominance of Linear 2-Coordination in Mercury Chemistry: Quasirelativistic and Nonrelativistic ab Initio Pseudopotential Study of $(\text{HgX}_2)_2$ (X = F, Cl, Br, I, H). <i>Inorganic Chemistry</i> , 1994, 33, 2555-2564. | 1.9 | 92 |
| 49 | Relationships in the rotational barriers of all Group 14 ethane congeners $\text{H}_3\text{X}-\text{YH}_3$ (X, Y = C, Si, Ge, Sn). <i>Journal of the American Chemical Society</i> , 1992, 114, 6791-6797. | 6.6 | 90 |
| 50 | Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. <i>Chemical Physics Letters</i> , 1995, 235, 382-388. | 1.2 | 90 |
| 51 | ReSpect: Relativistic spectroscopy DFT program package. <i>Journal of Chemical Physics</i> , 2020, 152, 184101. | 1.2 | 90 |
| 52 | Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. <i>Journal of Chemical Physics</i> , 2004, 120, 2127-2139. | 1.2 | 89 |
| 53 | Local hybrid functionals: An assessment for thermochemical kinetics. <i>Journal of Chemical Physics</i> , 2007, 127, 194102. | 1.2 | 87 |
| 54 | Origin of the Unique Stability of Condensed-Phase Hg^{2+} . An ab Initio Investigation of M I and M II Species (M = Zn, Cd, Hg). <i>Inorganic Chemistry</i> , 1994, 33, 4179-4185. | 1.9 | 86 |

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| 55 | Reversible [4Fe-3S] cluster morphing in an O ₂ -tolerant [NiFe] hydrogenase. <i>Nature Chemical Biology</i> , 2014, 10, 378-385. | 3.9 | 85 |
| 56 | Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. <i>Journal of Chemical Physics</i> , 2012, 136, 014111. | 1.2 | 83 |
| 57 | Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4189-4203. | 2.3 | 83 |
| 58 | Scalar Relativistic Effects on ¹⁷ O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. <i>Journal of the American Chemical Society</i> , 1995, 117, 1851-1852. | 6.6 | 82 |
| 59 | The calculation of ¹⁷ O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. <i>Journal of Chemical Physics</i> , 1997, 106, 9201-9212. | 1.2 | 81 |
| 60 | Giant Spin-Orbit Effects on NMR Shifts in Diamagnetic Actinide Complexes: Guiding the Search of Uranium(VI) Hydride Complexes in the Correct Spectral Range. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10884-10888. | 7.2 | 81 |
| 61 | Oxidation State +IV in Group 12 Chemistry. Ab Initio Study of Zinc(IV), Cadmium(IV), and Mercury(IV) Fluorides. <i>Inorganic Chemistry</i> , 1994, 33, 2122-2131. | 1.9 | 80 |
| 62 | The Structure of XeF ₆ and of Compounds Isoelectronic with It. A Challenge to Computational Chemistry and to the Qualitative Theory of the Chemical Bond. <i>Journal of the American Chemical Society</i> , 1996, 118, 11939-11950. | 6.6 | 79 |
| 63 | The Structure of Hexamethyltungsten, W(CH ₃) ₆ : Distorted Trigonal Prismatic with C ₃ Symmetry. <i>Journal of the American Chemical Society</i> , 1996, 118, 3018-3024. | 6.6 | 78 |
| 64 | Mixed-Valence Ruthenium Complexes Rotating through a Conformational Robin-Day Continuum. <i>Chemistry - A European Journal</i> , 2014, 20, 6895-6908. | 1.7 | 76 |
| 65 | Mechanism of the cooperative Si-H bond activation at Ru-S bonds. <i>Chemical Science</i> , 2015, 6, 4324-4334. | 3.7 | 76 |
| 66 | Density Functional Calculations of ⁵⁵ Mn, ¹⁴ N and ¹³ C Electron Paramagnetic Resonance Parameters Support an Energetically Feasible Model System for the S ₂ State of the Oxygen-Evolving Complex of Photosystem II. <i>Chemistry - A European Journal</i> , 2010, 16, 10424-10438. | 1.7 | 73 |
| 67 | Structure of the Oxygen-Rich Cluster Cation Al ₂ O ₇ ⁺ and its Reactivity toward Methane and Water. <i>Journal of the American Chemical Society</i> , 2011, 133, 16930-16937. | 6.6 | 73 |
| 68 | Density functional analysis of ¹³ C and ¹ H chemical shifts and bonding in mercurimethanes and organomercury hydrides: The role of scalar relativistic, spin-orbit, and substituent effects. <i>Journal of Chemical Physics</i> , 1998, 108, 3648-3659. | 1.2 | 72 |
| 69 | Relativistic two-component calculations of electronic g-tensors that include spin polarization. <i>Journal of Chemical Physics</i> , 2005, 123, 244103. | 1.2 | 72 |
| 70 | The Family of Ferrocene-Stabilized Silylium Ions: Synthesis, ²⁹ Si-NMR Characterization, Lewis Acidity, Substituent Scrambling, and Quantum-Chemical Analyses. <i>Chemistry - A European Journal</i> , 2013, 19, 16579-16594. | 1.7 | 69 |
| 71 | Efficient Self-Consistent Implementation of Local Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1540-1548. | 2.3 | 69 |
| 72 | Towards improved local hybrid functionals by calibration of exchange-energy densities. <i>Journal of Chemical Physics</i> , 2014, 141, 204101. | 1.2 | 68 |

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| 73 | A Density Functional Study of EPR Parameters for Vanadyl Complexes Containing Schiff Base Ligands. <i>Journal of Physical Chemistry B</i> , 2001, 105, 12644-12652. | 1.2 | 67 |
| 74 | Validation study of meta-GGA functionals and of a model exchange correlation potential in density functional calculations of EPR parameters. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5467-5474. | 1.3 | 67 |
| 75 | A Rare Uranyl(VI) Alkyl Ate Complex [Li(DME) _{1.5}] ₂ [UO ₂ (CH ₂ SiMe ₃) ₄] and Its Comparison with a Homoleptic Uranium(VI) Hexaalkyl. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3259-3263. | 7.2 | 67 |
| 76 | [Pb ₅ {Mo(CO) ₃] ₂] ⁴⁺ : A Complex Containing a Planar Pb ₅ Unit. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2092-2096. | 7.2 | 66 |
| 77 | Calculation of zero-field splitting parameters: Comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach. <i>Journal of Chemical Physics</i> , 2006, 125, 054110. | 1.2 | 66 |
| 78 | Combined Spectroscopic and Quantum Chemical Study of <i>trans</i> -Ru(Câ% ₆ H ₄) ₂ (dppe) ₂ and <i>trans</i> -Ru(Câ% ₆ H ₄) ₂ (Câ% ₆ H ₄) ₂ (<i>n</i> = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. <i>Organometallics</i> , 2014, 33, 4947-4963. | 1.1 | 66 |
| 79 | Systematic Experimental and Quantum Chemical Investigation into the Structures, the Stability, and the Spectroscopic Properties of Alkylindium(I) Compounds: Tetrameric In ₄ [C(SiMeRRâ€)3] ₄ versus Monomeric InC(SiMeRRâ€)3 Derivatives. <i>Organometallics</i> , 1998, 17, 5009-5017. | 1.1 | 64 |
| 80 | From local hybrid functionals to localized local hybrid potentials: Formalism and thermochemical tests. <i>Journal of Chemical Physics</i> , 2006, 124, 204102. | 1.2 | 64 |
| 81 | Formation and Characterization of the Iridium Tetroxide Molecule with Iridium in the Oxidation State +VIII. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 7879-7883. | 7.2 | 64 |
| 82 | Squaraine Dyes as Efficient Coupling Bridges between Triarylamine Redox Centres. <i>Chemistry - A European Journal</i> , 2011, 17, 14147-14163. | 1.7 | 64 |
| 83 | Synthesis and Bonding in Carbene Complexes of an Unsymmetrical Dilithio Methandiide: A Combined Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2013, 19, 16729-16739. | 1.7 | 64 |
| 84 | Gaseous Mercury(IV) Fluoride, HgF ₄ : An Ab Initio Study. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 861-863. | 4.4 | 63 |
| 85 | Density Functional Study of EPR Parameters and Spin-Density Distribution of Azurin and Other Blue Copper Proteins. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8290-8304. | 1.2 | 63 |
| 86 | Spin Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spin Orbit Operators. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5026-5033. | 1.1 | 62 |
| 87 | Refining the Interpretation of Near-Infrared Band Shapes in a Polyynediyl Molecular Wire. <i>Chemistry - A European Journal</i> , 2013, 19, 9780-9784. | 1.7 | 61 |
| 88 | Multifrequency EPR Study and Density Functional g-Tensor Calculations of Persistent Organorhenium Radical Complexes. <i>Journal of the American Chemical Society</i> , 2002, 124, 10563-10571. | 6.6 | 60 |
| 89 | Ro-Vibrational Corrections to NMR Parameters. , 2004, , 153-173. | | 60 |
| 90 | A Relativistic Quantum-Chemical Analysis of the <i>trans</i> Influence on ¹ H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 7199-7208. | 1.9 | 60 |

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| 91 | Ab Initio Molecular Dynamics Simulations and g-Tensor Calculations of Aqueous Benzosemiquinone Radical Anion: Effects of Regular and π -Stacked Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2004, 126, 9854-9861. | 6.6 | 59 |
| 92 | Do low-coordinated Group 1-3 cations Mn+Lm (Mn+ = potassium, rubidium cesium, calcium, strontium,) Tj ETQq0 0 0 rgBT /Overlock 10 noble-gas electron configuration favor regular or abnormal shapes?. <i>The Journal of Physical Chemistry</i> , 1992, 96, 7316-7323. | 2.9 | 57 |
| 93 | Understanding Substituent Effects on ^{29}Si Chemical Shifts and Bonding in Disilenes. <i>A Quantum Chemical Analysis</i> . <i>Organometallics</i> , 2003, 22, 2442-2449. | 1.1 | 57 |
| 94 | Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method. <i>Chemical Physics Letters</i> , 2004, 396, 268-276. | 1.2 | 57 |
| 95 | Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4984-4996. | 2.3 | 57 |
| 96 | Has AuF7 Been Made?. <i>Inorganic Chemistry</i> , 2006, 45, 1228-1234. | 1.9 | 56 |
| 97 | Formal Oxidation State versus Partial Charge – A Comment. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 986-986. | 4.4 | 55 |
| 98 | The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density. <i>Chemical Physics Letters</i> , 2003, 381, 495-504. | 1.2 | 55 |
| 99 | Validation of density functional methods for computing structures and energies of mercury(IV) complexes. Electronic supplementary information (ESI) available: Structure of transition state for HgH4 dissociation and tables with CP-connections and transition state structures. See http://www.rsc.org/suppdata/cp/b3/b315019d/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1122. | 1.3 | 55 |
| 100 | Structure of the Nucleotide Radical Formed during Reaction of CDP/TTP with the E441Q- Δ 2 of <i>E. coli</i> Ribonucleotide Reductase. <i>Journal of the American Chemical Society</i> , 2009, 131, 200-211. | 6.6 | 55 |
| 101 | The Nonoctahedral Structures of d0, d1, and d2 Hexamethyl Complexes. <i>Chemistry - A European Journal</i> , 1998, 4, 1678-1686. | 1.7 | 54 |
| 102 | The Function of Photosystem I. Quantum Chemical Insight into the Role of Tryptophan-Quinone Interactions. <i>Biochemistry</i> , 2002, 41, 2895-2900. | 1.2 | 54 |
| 103 | Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin-Spin Coupling., 2004, , 209-226. | | 54 |
| 104 | Relativistic Effects on NMR Chemical Shifts. <i>Theoretical and Computational Chemistry</i> , 2004, 14, 552-597. | 0.2 | 54 |
| 105 | Jacobsen's Catalyst for Hydrolytic Kinetic Resolution: Structure Elucidation of Paramagnetic Co(III) Salen Complexes in Solution via Combined NMR and Quantum Chemical Studies. <i>Journal of the American Chemical Society</i> , 2009, 131, 4172-4173. | 6.6 | 54 |
| 106 | Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4226-4237. | 2.3 | 54 |
| 107 | A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5645-5657. | 2.3 | 54 |
| 108 | A Trimetallic Gold Boride Complex with a Fluxional Gold-Boron Bond. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9735-9738. | 7.2 | 53 |

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| 109 | Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transition-Metal Carbonyl Complexes. <i>Chemistry - A European Journal</i> , 1996, 2, 24-30. | 1.7 | 52 |
| 110 | First-Principles Calculations of Paramagnetic NMR Shifts. , 2004, , 325-338. | | 52 |
| 111 | Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method with a finite-size nucleus model. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4079-4085. | 1.3 | 52 |
| 112 | Synthesis, Reactivity, and Electronic Structure of [Vanadoarenophanes: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 11376-11393. | 6.6 | 52 |
| 113 | The Cluster Anion Si ₉₄ ⁴⁻ . <i>Angewandte Chemie - International Edition</i> , 1998, 37, 2359-2361. | 7.2 | 51 |
| 114 | Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14713-14717. | 7.2 | 51 |
| 115 | Predicting the Localized/Delocalized Character of Mixed-Valence Diquinone Radical Anions. Toward the Right Answer for the Right Reason. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10629-10637. | 1.1 | 50 |
| 116 | Structure of the Nitrogen-Centered Radical Formed during Inactivation of E. coli Ribonucleotide Reductase by 2-Azido-2-deoxyuridine-5-diphosphate: A Trapping of the 3-Ketonucleotide. <i>Journal of the American Chemical Society</i> , 2005, 127, 7729-7738. | 6.6 | 49 |
| 117 | Understanding Structure and Bonding in Early Actinide 6d ⁰ 5f ⁰ MX ₆ q (M = Th-Np; X = H, F) Complexes in Comparison with Their Transition Metal 5d ⁰ Analogues. <i>Journal of the American Chemical Society</i> , 2005, 127, 2591-2599. | 6.6 | 49 |
| 118 | Diphosphines with Strongly Polarized P-P Bonds: Hybrids between Covalent Molecules and Donor-Acceptor Adducts with Flexible Molecular Structures. <i>Journal of the American Chemical Society</i> , 2009, 131, 10763-10774. | 6.6 | 49 |
| 119 | Four-Component Relativistic Density Functional Theory Calculations of EPR- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12892-12905. | 1.1 | 49 |
| 120 | Solid-State Nuclear Magnetic Resonance Spectroscopic and Quantum Chemical Investigation of ¹³ C and ¹⁷ O Chemical Shift Tensors, ¹⁷ O Nuclear Quadrupole Coupling Tensors, and Bonding in Transition-Metal Carbonyl Complexes and Clusters. <i>Journal of the American Chemical Society</i> , 1998, 120, 4771-4783. | 6.6 | 48 |
| 121 | The PI ₄ ⁺ cation has an extremely large negative ³¹ P nuclear magnetic resonance chemical shift, due to spin-orbit coupling: A quantum-chemical prediction and its confirmation by solid-state nuclear magnetic resonance spectroscopy. <i>Journal of Chemical Physics</i> , 1999, 110, 3897-3902. | 1.2 | 46 |
| 122 | Phosphorus Chemical Shifts in a Nucleic Acid Backbone from Combined Molecular Dynamics and Density Functional Calculations. <i>Journal of the American Chemical Society</i> , 2010, 132, 17139-17148. | 6.6 | 45 |
| 123 | From Silylone to an Isolable Monomeric Silicon Disulfide Complex. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 10254-10257. | 7.2 | 45 |
| 124 | New Zwitterionic Spirocyclic Si-Silicates with an Si ₄ C Skeleton (X = S, O) Containing Two Ligands of the Dithiolato(2-) or Diolato(2-) Type: A Synthesis, Structure, and Bonding Situation. <i>Organometallics</i> , 2003, 22, 4104-4110. | 1.1 | 44 |
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