Martin Kaupp

List of Publications by Year
in descending order

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377 papers	18,026 citations	14124 69 h-index	30277 107 g-index
418 all docs	418 docs citations	418 times ranked	12273 citing authors

#	Article	IF	Citations
1	A Look at Realâ€World Transitionâ€Metal Thermochemistry and Kinetics with Local Hybrid Functionals. Israel Journal of Chemistry, 2023, 63, .	1.0	8
2	Competition for Hydride Between Silicon and Boron: Synthesis and Characterization of a Hydroboraneâ€Stabilized Silylium Ion. Chemistry - A European Journal, 2022, 28, e202104464.	1.7	7
3	Investigation of Molecular Iridium Fluorides IrF _n (n =1â€“6): A Combined Matrixâ€Isolation and Quantumâ€Chemical Study. Chemistry - A European Journal, 2022, , e202104005.	1.7	2
4	Synthesis of Intramolecular P/Alâ€Based Frustrated Lewis Pairs via Aluminumâ€Tinâ€Exchange and their Reactivity toward CO₂. Chemistry - A European Journal, 2022, 28, .	1.7	10
5	Synthesis, Reactivity, and Bonding of Gold(I) Fluoridoâ€“Phosphine Complexes. Inorganic Chemistry, 2022, 61, 357-367.	1.9	7
6	Systematic Evaluation of Modern Density Functional Methods for the Computation of NMR Shifts of 3d Transition-Metal Nuclei. Journal of Chemical Theory and Computation, 2022, 18, 273-292.	2.3	11
7	Reaction Entropies in Solution from Analytical Three-Dimensional Reference Interaction Site Model Derivatives with Application to Redox and Spin-Crossover Processes. Journal of Physical Chemistry A, 2022, 126, 3708-3716.	1.1	3
8	Tetrylâ€Tetrylene Addition to Phenylacetylene. Chemistry - A European Journal, 2021, 27, 4691-4699.	1.7	4
9	Iron Versus Ruthenium: Evidence for the Distinct Differences in the Electronic Structures of Hexa-1,3,5-triyn-1,6-diyl-bridged Complexes [Cp*(dppe)M}{Î¼-(Câ‰¡C)₃}{M(dppe)Cp*}]⁺ (M = Fe, Ru). Organometallics, 2021, 40, 346-357.	2.1	15
10	Effect of the Current Dependence of Tau-Dependent Exchange-Correlation Functionals on Nuclear Shielding Calculations. Journal of Chemical Theory and Computation, 2021, 17, 1469-1479.	2.3	25
11	The Supramolecular Structural Chemistry of Pentafluorosulfanyl and Tetrafluorosulfanylene Compounds. Chemistry - A European Journal, 2021, 27, 6086-6093.	1.7	11
12	Implementation and Validation of Local Hybrid Functionals with Calibrated Exchange-Energy Densities for Nuclear Shielding Constants. Journal of Physical Chemistry A, 2021, 125, 2697-2707.	1.1	13
13	Reliable TDDFT Protocol Based on a Local Hybrid Functional for the Prediction of Vibronic Phosphorescence Spectra Applied to Tris(2,2â€²-bipyridine)-Metal Complexes. Journal of Physical Chemistry A, 2021, 125, 7099-7110.	1.1	13
14	Matrix Isolation Spectroscopic and Relativistic Quantum Chemical Study of Molecular Platinum Fluorides PtF n (n =1â€“6) Reveals Magnetic Bistability of PtF 4. Chemistry - A European Journal, 2021, 27, 13642-13650.	1.7	3
15	Assessment of hybrid functionals for singlet and triplet excitations: Why do some local hybrid functionals perform so well for triplet excitation energies?. Journal of Chemical Physics, 2021, 155, 124108.	1.2	14
16	Platinum Indolylphosphine Fluorido and Polyfluorido Complexes: An Interplay between Cyclometallation, Fluoride Migration, and Hydrogen Bonding. Chemistry - A European Journal, 2021, 27, 14287-14298.	1.7	10
17	Novel synthetic pathway for the production of phosgene. Science Advances, 2021, 7, eabj5186.	4.7	19
18	Hydroxy-bridged resting states of a [NiFe]-hydrogenase unraveled by cryogenic vibrational spectroscopy and DFT computations. Chemical Science, 2021, 12, 2189-2197.	3.7	17

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19	Local hybrid functionals augmented by a strong-correlation model. Journal of Chemical Physics, 2021, 155, 144101.	1.2	12
20	Spin-state control of cobalt(ii) and iron(ii) complexes with click-derived tripodal ligands through non-covalent and fluorine-specific interactions. Dalton Transactions, 2021, , .	1.6	2
21	Extended Benchmark Set of Main-Group Nuclear Shielding Constants and NMR Chemical Shifts and Its Use to Evaluate Modern DFT Methods. Journal of Chemical Theory and Computation, 2021, 17, 7602-7621.	2.3	37
22	An Efficient Coupled-Perturbed Kohnâ€“Sham Implementation of NMR Chemical Shift Computations with Local Hybrid Functionals and Gauge-Including Atomic Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 931-943.	2.3	34
23	Noncollinear Relativistic Two-Component X2C Calculations of Hyperfine Couplings Using Local Hybrid Functionals. Importance of the High-Density Coordinate Scaling Limit. Journal of Chemical Theory and Computation, 2020, 16, 314-325.	2.3	19
24	Electronic States of 2,3-Diamino-1,4-naphthoquinone and Its N-Alkylated Derivatives. Journal of Physical Chemistry C, 2020, 124, 60-69.	1.5	12
25	Nuclear Spinâ€“Spin Couplings: Efficient Evaluation of Exact Exchange and Extension to Local Hybrid Functionals. Journal of Physical Chemistry A, 2020, 124, 8529-8539.	1.1	17
26	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Leftâ€“Right Correlation. Journal of Chemical Theory and Computation, 2020, 16, 5645-5657.	2.3	54
27	Validation of Local Hybrid Functionals for Excited States: Structures, Fluorescence, Phosphorescence, and Vibronic Spectra. Journal of Chemical Theory and Computation, 2020, 16, 5821-5834.	2.3	21
28	Hyperfine-Coupling Tensors from Projected Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2020, 16, 6222-6235.	2.3	3
29	Evaluation of an Efficient 3D-RISM-SCF Implementation as a Tool for Computational Spectroscopy in Solution. Journal of Physical Chemistry A, 2020, 124, 7439-7452.	1.1	13
30	Picometer Resolution Structure of the Coordination Sphere in the Metal-Binding Site in a Metalloprotein by NMR. Journal of the American Chemical Society, 2020, 142, 16757-16765.	6.6	33
31	Evaluation of Local Hybrid Functionals for Electric Properties: Dipole Moments and Static and Dynamic Polarizabilities. Journal of Physical Chemistry A, 2020, 124, 8346-8358.	1.1	15
32	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	1.2	90
33	Verbesserter Zugang zu organisch lÃ¶slichen Diâ€•und Tetrafluoridochlorat(I/III)â€Salzen. Angewandte Chemie, 2020, 132, 16136-16140.	1.6	8
34	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
35	Improved Access to Organoâ€Soluble Diâ€•and Tetrafluoridochlorate(I)/(III) Salts. Angewandte Chemie - International Edition, 2020, 59, 16002-16006.	7.2	14
36	Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. Chemical Reviews, 2020, 120, 7065-7103.	23.0	113

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37	Covalent vs Charge-Shift Nature of the Metalâ€“Metal Bond in Transition Metal Complexes: A Unified Understanding. Journal of the American Chemical Society, 2020, 142, 12277-12287.	6.6	37
38	A four-parameter system for rationalising the electronic properties of transition metalâ€“radical ligand complexes. Dalton Transactions, 2020, 49, 9735-9742.	1.6	7
39	Câ€“P vs Câ€“H Bond Cleavage of Triphenylphosphine at Platinum(0): Mechanism of Formation, Reactivity, Redox Chemistry, and NMR Chemical Shift Calculations of a Î¼-Phosphanido Diplatinum(II) Platform. Organometallics, 2020, 39, 443-452.	1.1	7
40	Stable Actinide Ï€ Complexes of a Neutral 1,4â€Diborabenzene. Angewandte Chemie - International Edition, 2020, 59, 13109-13115.	7.2	15
41	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1378.	6.2	95
42	Insights from 125Te and 57Fe nuclear resonance vibrational spectroscopy: a [4Feâ€“4Te] cluster from two points of view. Chemical Science, 2019, 10, 7535-7541.	3.7	5
43	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2019, 15, 5508-5522.	2.3	21
44	Asymmetry in the Ligand Coordination Sphere of the [FeFe] Hydrogenase Active Site Is Reflected in the Magnetic Spin Interactions of the Aza-propanedithiolate Ligand. Journal of Physical Chemistry Letters, 2019, 10, 6794-6799.	2.1	22
45	Density Functional Calculations of Electron Paramagnetic Resonance g- and Hyperfine-Coupling Tensors Using the Exact Two-Component (X2C) Transformation and Efficient Approximations to the Two-Electron Spinâ€“Orbit Terms. Journal of Physical Chemistry A, 2019, 123, 5660-5672.	1.1	20
46	Câˆ’H and Câˆ’F Bond Activation Reactions of Fluorinated Propenes at Rhodium: Distinctive Reactivity of the Refrigerant HFOâ€1234yf. Angewandte Chemie, 2019, 131, 10798-10802.	1.6	12
47	Quantum-chemical study of 7Li NMR shifts in the context of delithiation of paramagnetic lithium vanadium phosphate, Li3V2(PO4)3 (LVP). Solid State Nuclear Magnetic Resonance, 2019, 101, 89-100.	1.5	6
48	Câˆ’H and Câˆ’F Bond Activation Reactions of Fluorinated Propenes at Rhodium: Distinctive Reactivity of the Refrigerant HFOâ€1234yf. Angewandte Chemie - International Edition, 2019, 58, 10688-10692.	7.2	21
49	A Spectroscopic and Computationally Minimal Approach to the Analysis of Chargeâ€Transfer Processes in Conformationally Fluxional Mixedâ€Valence and Heterobimetallic Complexes. Chemistry - A European Journal, 2019, 25, 8837-8853.	1.7	19
50	A Silyleneâ€“Borane Lewis Pair as a Tool for Trapping a Water Molecule: Silanol Formation and Dehydrogenation. Chemistry - A European Journal, 2019, 25, 4678-4682.	1.7	8
51	Computation of NMR Shifts for Paramagnetic Solids Including Zero-Field-Splitting and Beyond-DFT Approaches. Application to LiMPO₄ (M = Mn, Fe, Co, Ni) and MPO₄ (M = Fe, Co). Journal of Physical Chemistry C, 2019, 123, 8387-8405.	1.5	21
52	Hubbard Trimer with Spinâ€“Orbit Coupling: Hartreeâ€“Fock Solutions, (Non)Collinearity, and Anisotropic Spin Hamiltonian. Journal of Physical Chemistry A, 2019, 123, 2361-2378.	1.1	5
53	Activation of tetrafluoropropenes by rhodium(<scp>i</scp>) germyl and silyl complexes. Faraday Discussions, 2019, 220, 328-349.	1.6	8
54	Characterization of hydrogen-substituted silylium ions in the condensed phase. Science, 2019, 365, 168-172.	6.0	32

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55	Ligand Effects on the Reactivity of [CoX]+ (Xâ€‰=â€‰CN, F, Cl, Br, O, OH) Towards CO2: Gas-Phase Generation of the Elusive Cyanoformate by [Co(CN)]+ and [Fe(CN)]+. Topics in Catalysis, 2018, 61, 575-584.	1.3	9
56	Quantum-Chemical Approach to NMR Chemical Shifts in Paramagnetic Solids Applied to LiFePO₄ and LiCoPO₄. Journal of Physical Chemistry Letters, 2018, 9, 1480-1484.	2.1	25
57	Noncollinear Two-Component Quasirelativistic Description of Spin Interactions in Exchange-Coupled Systems. Mapping Generalized Broken-Symmetry States to Effective Spin Hamiltonians. Journal of Chemical Theory and Computation, 2018, 14, 1267-1276.	2.3	3
58	Exact Mapping from Manyâ€Spin Hamiltonians to Giantâ€Spin Hamiltonians. Chemistry - A European Journal, 2018, 24, 4689-4702.	1.7	11
59	Probing Interactions of N-Donor Molecules with Open Metal Sites within Paramagnetic Cr-MIL-101: A Solid-State NMR Spectroscopic and Density Functional Theory Study. Journal of the American Chemical Society, 2018, 140, 2135-2144.	6.6	41
60	Iron versus Ruthenium: Clarifying the Electronic Differences between Prototypical Mixed-Valence Organometallic Butadiyndiyl Bridged Molecular Wires. Organometallics, 2018, 37, 1432-1445.	1.1	44
61	Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. Journal of Chemical Theory and Computation, 2018, 14, 377-394.	2.3	34
62	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 5653-5672.	2.3	35
63	MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. Journal of Chemical Theory and Computation, 2018, 14, 3512-3523.	2.3	20
64	InnenrÃ¼cktitelbild: An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone (Angew. Chem. 7/2017). Angewandte Chemie, 2017, 129, 1957-1957.	1.6	0
65	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. Angewandte Chemie, 2017, 129, 1920-1923.	1.6	20
66	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. Angewandte Chemie - International Edition, 2017, 56, 1894-1897.	7.2	44
67	Internal Dynamics of the 3-Pyrroline-N-Oxide Ring in Spin-Labeled Proteins. Journal of Physical Chemistry Letters, 2017, 8, 1113-1117.	2.1	2
68	DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids. Physical Review B, 2017, 95, .	1.1	31
69	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. Coordination Chemistry Reviews, 2017, 344, 355-362.	9.5	99
70	Taming Silicon Congeners of CO and CO₂: Synthesis of Monomeric Si^{II} and Si^{IV} Chalcogenide Complexes. Angewandte Chemie - International Edition, 2017, 56, 6298-6301.	7.2	23
71	Taming Silicon Congeners of CO and CO₂: Synthesis of Monomeric Si^{II} and Si^{IV} Chalcogenide Complexes. Angewandte Chemie, 2017, 129, 6395-6398.	1.6	8
72	Metalâ€Dependent Strengthening and Weakening of Mâ^'H and Mâ^'C Bonds by an Oxo Ligand: Thermal Gasâ€Phase Activation of Methane by [OMH]⁺ and [MH]⁺ (M=Mo, Ti). Chemistry - A European Journal, 2017, 23, 12346-12352.	1.7	7

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73	Insights into transâ€Ligand and Spinâ€Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transitionâ€Metal Complexes. Chemistry - A European Journal, 2017, 23, 9790-9803.	1.7	42
74	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. Journal of Chemical Theory and Computation, 2017, 13, 4984-4996.	2.3	57
75	On the Electronic Origin of Remarkable Ligand Effects on the Reactivities of [NiL]⁺ Complexes (L=C₆H₅, C₅H₄N, CN) towards Methane. Chemistry - A European Journal, 2017, 23, 14430-14433.	1.7	6
76	Reactivity of the Sterically Demanding Siloxanediol Mes₂Si(OH)(Î¼â€O)Si(OH)Mes₂ Towards Water and Ether Molecules. Chemistry - A European Journal, 2017, 23, 13964-13972.	1.7	6
77	Insights into trans -Ligand and Spin-Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transition-Metal Complexes. Chemistry - A European Journal, 2017, 23, 9702-9702.	1.7	5
78	Four-Component Relativistic Density Functional Calculations of EPR Parameters for Model Complexes of Tungstoenzymes. Journal of Physical Chemistry A, 2017, 121, 9106-9117.	1.1	5
79	A high-spin square planar iron(<scp>ii</scp>)-siloxide and its tetrahedral allogon â€“ structural and spectroscopic models of Fe-zeolite sites. Chemical Communications, 2017, 53, 8081-8084.	2.2	18
80	Construction of Giantâ€Spin Hamiltonians from Manyâ€Spin Hamiltonians by Thirdâ€Order Perturbation Theory and Application to an Fe₃Cr Singleâ€Molecule Magnet. Chemistry - A European Journal, 2016, 22, 6853-6862.	1.7	6
81	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. Journal of Chemical Physics, 2016, 144, 074106.	1.2	117
82	New approaches for the calibration of exchange-energy densities in local hybrid functionals. Physical Chemistry Chemical Physics, 2016, 18, 21133-21144.	1.3	43
83	Electron transfer pathways in mixedâ€valence paracyclophaneâ€bridged bisâ€triarylamine radical cations. Journal of Computational Chemistry, 2016, 37, 93-102.	1.5	15
84	Completing the Heterocubane Family [Cp*AlE]₄ (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al]₄: Density Functional Theory Calculations of [Cp*AlE]₄ and Reactivity of [Cp*AlO]₄ toward Hydrolysis. Inorganic Chemistry, 2016, 55, 4915-4923.	1.9	38
85	Paramagnetic NMR of Phenolic Oxime Copper Complexes: A Joint Experimental and Density Functional Study. Chemistry - A European Journal, 2016, 22, 15328-15339.	1.7	22
86	Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. Journal of Chemical Theory and Computation, 2016, 12, 4254-4262.	2.3	33
87	Tracking Transient Conformational States of T4 Lysozyme at Room Temperature Combining X-ray Crystallography and Site-Directed Spin Labeling. Journal of the American Chemical Society, 2016, 138, 12868-12875.	6.6	13
88	Understanding Thermodynamic and Spectroscopic Properties of Tetragonal Mn12Single-Molecule Magnets from Combined Density Functional Theory/Spin-Hamiltonian Calculations. Journal of Physical Chemistry A, 2016, 120, 6864-6879.	1.1	17
89	Rational Control of Conformational Distributions and Mixedâ€Valence Characteristics in Diruthenium Complexes. Chemistry - A European Journal, 2016, 22, 16138-16146.	1.7	38
90	On the Activation of Methane and Carbon Dioxide by [HTaO]⁺ and [TaOH]⁺ in the Gas Phase: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 10581-10589.	1.7	16

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91	[Al₂O₄]^{â”}, a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2016, 12, 3796-3806.	2.3	20
92	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717.	7.2	51
93	Giant spinâ€“orbit effects on ¹H and ¹³C NMR shifts for uranium(<scp>vi</scp>) complexes revisited: role of the exchangeâ€“correlation response kernel, bonding analyses, and new predictions. Physical Chemistry Chemical Physics, 2016, 18, 30462-30474.	1.3	42
94	Tetrakis(ferrocenylethynyl)ethene: Synthesis, (Spectro)electrochemical and quantum chemical characterisation. Journal of Organometallic Chemistry, 2016, 821, 40-47.	0.8	11
95	Wavelength selective polymer network formation of end-functional star polymers. Chemical Communications, 2016, 52, 1975-1978.	2.2	43
96	Gauge effects in local hybrid functionals evaluated for weak interactions and the GMTKN30 test set. Molecular Physics, 2016, 114, 1118-1127.	0.8	26
97	The MÃ¶ssbauer Parameters of the Proximal Cluster of Membrane-Bound Hydrogenase Revisited: A Density Functional Theory Study. Journal of Chemical Theory and Computation, 2016, 12, 174-187.	2.3	11
98	Mechanistic aspects of CO2 activation mediated by phenyl yttrium cation: A combined experimental/theoretical study. Journal of Catalysis, 2016, 343, 68-74.	3.1	9
99	Design of exchange-correlation functionals through the correlation factor approach. Journal of Chemical Physics, 2015, 143, 144102.	1.2	30
100	Biomimetic [2Feâ€2S] Clusters with Extensively Delocalized Mixedâ€Valence Iron Centers. Angewandte Chemie - International Edition, 2015, 54, 12506-12510.	7.2	35
101	From Silylone to an Isolable Monomeric Silicon Disulfide Complex. Angewandte Chemie - International Edition, 2015, 54, 10254-10257.	7.2	45
102	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€“Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	1.1	49
103	A Relativistic Quantum-Chemical Analysis of the trans Influence on ¹H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. Inorganic Chemistry, 2015, 54, 7199-7208.	1.9	60
104	Efficient Self-Consistent Implementation of Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2015, 11, 1540-1548.	2.3	69
105	Relativistic and Solvation Effects on the Stability of Gold(III) Halides in Aqueous Solution. Inorganic Chemistry, 2015, 54, 9869-9875.	1.9	14
106	Mechanism of the cooperative Siâ€“H bond activation at Ruâ€“S bonds. Chemical Science, 2015, 6, 4324-4334.	3.7	76
107	Controlled ligand distortion and its consequences for structure, symmetry, conformation and spin-state preferences of iron(<scp>ii</scp>) complexes. Dalton Transactions, 2015, 44, 19232-19247.	1.6	12
108	Cross-Conjugated Systems Based On An (E)-Hexa-3-en-1,5-diyne-3,4-diyl Skeleton: Spectroscopic and Spectroelectrochemical Investigations. Journal of Organic Chemistry, 2015, 80, 11501-11512.	1.7	7

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109	Correlations between metal spin states and vibrational spectra ofÂaÂtrinuclear Fe(II) complex exhibiting spin crossover. Journal of Molecular Structure, 2015, 1101, 8-13.	1.8	2
110	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4226-4237.	2.3	54
111	Validation of the Direct-COSMO-RS Solvent Model for Dielsâ€“Alder Reactions in Aqueous Solution. Journal of Chemical Theory and Computation, 2015, 11, 111-121.	2.3	13
112	Synthesis and redox properties of mono-, di- and tri-metallic platinum-ethynyl complexes based on the trans-Pt(C6H4N{C6H4OCH3-4}2)(C CR)(PPh3)2 motif. Polyhedron, 2015, 86, 31-42.	1.0	6
113	Communication: A non-empirical correlation factor model for the exchange-correlation energy. Journal of Chemical Physics, 2014, 141, 111102.	1.2	34
114	On Ammonia Binding to the Oxygenâ€Evolving Complex of Photosystemâ€…II: A Quantum Chemical Study. Chemistry - A European Journal, 2014, 20, 7300-7308.	1.7	33
115	Reversible [4Fe-3S] cluster morphing in an O2-tolerant [NiFe] hydrogenase. Nature Chemical Biology, 2014, 10, 378-385.	3.9	85
116	Ligand spheres in asymmetric hetero Dielsâ€“Alder reactions catalyzed by Cu(<scp>ii</scp>) box complexes: experiment and modeling. Dalton Transactions, 2014, 43, 698-705.	1.6	10
117	Quantum-chemical insights into mixed-valence systems: within and beyond the Robinâ€“Day scheme. Chemical Society Reviews, 2014, 43, 5067-5088.	18.7	168
118	Synthesis and vibrational spectroscopy of 57Fe-labeled models of [NiFe] hydrogenase: first direct observation of a nickelâ€“iron interaction. Chemical Communications, 2014, 50, 13469-13472.	2.2	12
119	A Combined Computational and Spectroelectrochemical Study of Platinum-Bridged Bis-Triarylamine Systems. Inorganic Chemistry, 2014, 53, 1544-1554.	1.9	43
120	Combined Spectroscopic and Quantum Chemical Study of [trans-Ru(Câ‰¡CC₆H₄R¹-4)₂(dppe)₂]ⁿ⁺ and [trans-Ru(Câ‰¡CC₆H₄R¹-4)(Câ‰¡CC₆H₄R²-4)(d (n = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. Organometallics, 2014, 33, 4947-4963.	1.1	66
121	Synthesis, Reactivity, and Electronic Structure of a Bioinspired Heterobimetallic [Ni(Î¼-S₂)Fe] Complex with Disulfur Monoradical character. Organometallics, 2014, 33, 3154-3162.	1.1	3
122	Mixedâ€Valence Ruthenium Complexes Rotating through a Conformational Robinâ€“Day Continuum. Chemistry - A European Journal, 2014, 20, 6895-6908.	1.7	76
123	Insight into the Mechanism of Carbonyl Hydrosilylation Catalyzed by Brookhartâ€™s Cationic Iridium(III) Pincer Complex. Journal of the American Chemical Society, 2014, 136, 6912-6915.	6.6	93
124	Towards improved local hybrid functionals by calibration of exchange-energy densities. Journal of Chemical Physics, 2014, 141, 204101.	1.2	68
125	Redox-Dependent Structural Transformations of the [4Fe-3S] Proximal Cluster in O₂-Tolerant Membrane-Bound [NiFe]-Hydrogenase: A DFT Study. Journal of the American Chemical Society, 2013, 135, 11809-11823.	6.6	29
126	Understanding Structure Formation in Organolithium Compounds: An Experimental and Quantumâ€Chemical Approach. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 2077-2085.	0.6	24

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127	From Bis(silylene) and Bis(germylene) Pincer-Type Nickel(II) Complexes to Isolable Intermediates of the Nickel-Catalyzed Sonogashira Cross-Coupling Reaction. Journal of the American Chemical Society, 2013, 135, 15617-15626.	6.6	232
128	A Heterobimetallic Approach To Stabilize the Elusive Disulfur Radical Trianion (â€œSubsulfideâ€) ${{m S}{{{{ullet}}3- hfill atop 2hfill}}}$. Chemistry - A European Journal, 2013, 19, 1246-1253.	1.7	9
129	Ab Initio and Density Functional Calculations of Electronic g-Tensors for Organic Radicals. Progress in Theoretical Chemistry and Physics, 2013, , 323-361.	0.2	3
130	The preparation, characterisation and electronic structures of 2,4-pentadiynylnitrile (cyanobutadiynyl) complexes. Dalton Transactions, 2013, 42, 4240.	1.6	7
131	Syntheses, Spectroelectrochemical Studies, and Molecular and Electronic Structures of Ferrocenyl Ene-diynes. Organometallics, 2013, 32, 6022-6032.	1.1	21
132	A Rare Uranyl(VI)â€“Alkyl Ate Complex [Li(DME)_{1.5}]₂[UO₂(CH₂SiMe₃)₄] and Its Comparison with a Homoleptic Uranium(VI)â€“Hexaalkyl. Angewandte Chemie - International Edition, 2013, 52, 3259-3263.	7.2	67
133	Refining the Interpretation of Nearâ€Infrared Band Shapes in a Polyynediyl Molecular Wire. Chemistry - A European Journal, 2013, 19, 9780-9784.	1.7	61
134	The Family of Ferroceneâ€Stabilized Silylium Ions: Synthesis,29Siâ€…NMR Characterization, Lewis Acidity, Substituent Scrambling, and Quantumâ€Chemical Analyses. Chemistry - A European Journal, 2013, 19, 16579-16594.	1.7	69
135	Synthesis and Bonding in Carbene Complexes of an Unsymmetrical Dilithio Methandiide: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2013, 19, 16729-16739.	1.7	64
136	Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. Journal of Chemical Physics, 2012, 136, 014111.	1.2	83
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