Florian Weigend

List of Publications by Year
in descending order

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171 papers	46,597 citations	43973 48 h-index	4535 171 g-index
194 all docs	194 docs citations	194 times ranked	27951 citing authors

#	Article	IF	Citations
1	Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. Physical Chemistry Chemical Physics, 2005, 7, 3297.	1.3	20,342
2	Accurate Coulomb-fitting basis sets for H to Rn. Physical Chemistry Chemical Physics, 2006, 8, 1057.	1.3	5,695
3	Auxiliary basis sets for main row atoms and transition metals and their use to approximate Coulomb potentials. Theoretical Chemistry Accounts, 1997, 97, 119-124.	0.5	3,172
4	RI-MP2: optimized auxiliary basis sets and demonstration of efficiency. Chemical Physics Letters, 1998, 294, 143-152.	1.2	2,469
5	Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. Journal of Chemical Physics, 2002, 116, 3175-3183.	1.2	1,671
6	RI-MP2: first derivatives and global consistency. Theoretical Chemistry Accounts, 1997, 97, 331-340.	0.5	1,347
7	CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. Journal of Chemical Physics, 2000, 113, 5154.	1.2	1,319
8	A fully direct RI-HF algorithm: Implementation, optimised auxiliary basis sets, demonstration of accuracy and efficiency. Physical Chemistry Chemical Physics, 2002, 4, 4285-4291.	1.3	1,185
9	Gaussian basis sets of quadruple zeta valence quality for atoms Hâ€“Kr. Journal of Chemical Physics, 2003, 119, 12753-12762.	1.2	946
10	Turbomole. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 91-100.	6.2	867
11	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
12	Hartreeâ€“Fock exchange fitting basis sets for H to Rn. Journal of Computational Chemistry, 2008, 29, 167-175.	1.5	552
13	A single-molecule diode. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 8815-8820.	3.3	437
14	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	2.3	280
15	The GW-Method for Quantum Chemistry Applications: Theory and Implementation. Journal of Chemical Theory and Computation, 2013, 9, 232-246.	2.3	216
16	Conductance of molecular wires and transport calculations based on density-functional theory. Physical Review B, 2004, 69, .	1.1	184
17	Approximated electron repulsion integrals: Cholesky decomposition versus resolution of the identity methods. Journal of Chemical Physics, 2009, 130, 164106.	1.2	176
18	Electronic transport through single conjugated molecules. Chemical Physics, 2002, 281, 113-125.	0.9	167

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19	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. Journal of Chemical Physics, 2013, 138, 184105.	1.2	158
20	Segmented contracted basis sets for one- and two-component Diracâ€“Fock effective core potentials. Journal of Chemical Physics, 2010, 133, 174102.	1.2	157
21	Slow Magnetic Relaxation in Trigonal-Planar Mononuclear Fe(II) and Co(II) Bis(trimethylsilyl)amido Complexesâ€”A Comparative Study. Inorganic Chemistry, 2014, 53, 1962-1974.	1.9	157
22	Self-consistent treatment of spinâ€“orbit interactions with efficient Hartreeâ€“Fock and density functional methods. Physical Chemistry Chemical Physics, 2008, 10, 1748.	1.3	145
23	Segmented Contracted Error-Consistent Basis Sets of Double- and Triple-Î¶ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3696-3705.	2.3	127
24	Theoretical study on clusters of magnesium. Physical Chemistry Chemical Physics, 2001, 3, 711-719.	1.3	122
25	Superatomic Orbitals under Spinâ€“Orbit Coupling. Journal of Physical Chemistry Letters, 2014, 5, 3286-3289.	2.1	122
26	Quasi-Particle Self-Consistent GW for Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2528-2541.	2.3	114
27	Binding energies of CO on gold cluster cations Aun+ (n=1â€“65): A radiative association kinetics study. Journal of Chemical Physics, 2005, 122, 104702.	1.2	105
28	Ortho-Chalcogenostannates as Ligands: Syntheses, Crystal Structures, Electronic Properties, and Magnetism of Novel Compounds Containing Ternary Anionic Substructures[M4(Î¼4-Se)(SnSe4)4]10â¯ (M=Mn, Zn, Cd, Hg),{[Hg4(Î¼4-Se)(SnSe4)3]6â¯}, or{[HgSnSe4]2â¯}. Chemistry - A European Journal, 2004, 10, 5147-5157.	1.7	99
29	Understanding of multimetallic cluster growth. Nature Communications, 2016, 7, 10480.	5.8	98
30	Error-Balanced Segmented Contracted Basis Sets of Double-Î¶ to Quadruple-Î¶ Valence Quality for the Lanthanides. Journal of Chemical Theory and Computation, 2012, 8, 4062-4068.	2.3	96
31	Quantum chemistry calculations for molecules coupled to reservoirs: Formalism, implementation, and application to benzenedithiol. Journal of Chemical Physics, 2007, 126, 174101.	1.2	94
32	Doped Semimetal Clusters: Ternary, Intermetalloid Anions [Ln@Sn₇Bi₇]^{4â€“} and [Ln@Sn₄Bi₉]^{4â€“} (Ln = La, Ce) with Adjustable Magnetic Properties. Journal of the American Chemical Society, 2012, 134, 1181-1191.	6.6	89
33	Unusual Syntheses, Structures, and Electronic Properties of Compounds Containing Ternary, T3-Type Supertetrahedral M/Sn/S Anions [M5Sn(Î¼3-S)4(SnS4)4]10-(M = Zn, Co). Inorganic Chemistry, 2005, 44, 5686-5695.	1.9	87
34	Main Group Metalâ€“Actinide Magnetic Coupling and Structural Response Upon U⁴⁺ Inclusion Into Bi, Tl/Bi, or Pb/Bi Cages. Journal of the American Chemical Society, 2016, 138, 9033-9036.	6.6	83
35	Seminumerical calculation of the Hartreeâ€“Fock exchange matrix: Application to twoâ€component procedures and efficient evaluation of local hybrid density functionals. Journal of Computational Chemistry, 2012, 33, 810-816.	1.5	68
36	Basis-set extensions for two-component spinâ€“orbit treatments of heavy elements. Physical Chemistry Chemical Physics, 2006, 8, 4862-4865.	1.3	65

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37	Making practical use of the pseudo-element concept: an efficient way to ternary intermetalloid clusters by an isoelectronic Pbâ^'â€“Bi combination. Chemical Communications, 2012, 48, 11295.	2.2	65
38	A N-Heterocyclic Carbene-Stabilized Coinage Metal-Chalcogenide Framework with Tunable Optical Properties. Journal of the American Chemical Society, 2017, 139, 14045-14048.	6.6	62
39	Substantial Ï€-aromaticity in the anionic heavy-metal cluster [Th@Bi12]4â^'. Nature Chemistry, 2021, 13, 149-155.	6.6	62
40	Structural Relaxation in Charged Metal Surfaces and Cluster Ions. Small, 2006, 2, 1497-1503.	5.2	59
41	Reactions of mixed silver-gold cluster cations AgmAun+ (m+n=4,5,6) with CO: Radiative association kinetics and density functional theory computations. Journal of Chemical Physics, 2006, 125, 104308.	1.2	56
42	Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. Journal of Chemical Physics, 2018, 148, 104110.	1.2	56
43	Binding energy and preferred adsorption sites of CO on gold and silverâ€“gold cluster cations: Adsorption kinetics and quantum chemical calculations. Faraday Discussions, 2008, 138, 393-406.	1.6	55
44	Error-consistent segmented contracted all-electron relativistic basis sets of double- and triple-zeta quality for NMR shielding constants. Physical Chemistry Chemical Physics, 2019, 21, 16658-16664.	1.3	55
45	Subtle Impact of Atomic Ratio, Charge and Lewis Basicity on Structure Selection and Stability: The Zintl Anion [(La@In₂Bi₁₁)(Î¼<i>â€<</i>Bi)₂(La@In₂Bi₁₁)]^{6â^'}. Chemistry - A European Journal, 2012, 18, 13589-13595.	1.7	54
46	Implementation of Two-Component Time-Dependent Density Functional Theory in TURBOMOLE. Journal of Chemical Theory and Computation, 2013, 9, 5341-5348.	2.3	53
47	Goldï£¿Gold Interactionâ€"Stannaborate [SnB11H11]2 Coordination Chemistry. Angewandte Chemie - International Edition, 2003, 42, 1501-1505.	7.2	50
48	Unusual 14â€Electron Fragments [Pd(Î·³â€Bi_{3â^'x}Pb_x)]^{(x+1)â^'} as Pseudo Lead Atoms in closoâ€[Pd@Pd₂Pb₁₀Bi₆]^{4â^'}. Angewandte Chemie - International Edition, 2013, 52, 13544-13548.	7.2	48
49	{[CuSn₅Sb₃]^{2â^'}}₂: A Dimer of Inhomogeneous Superatoms. Angewandte Chemie - International Edition, 2016, 55, 11775-11780.	7.2	48
50	Calculation of Magnetic Shielding Constants with meta-GGA Functionals Employing the Multipole-Accelerated Resolution of the Identity: Implementation and Assessment of Accuracy and Efficiency. Journal of Chemical Theory and Computation, 2018, 14, 191-197.	2.3	48
51	Red-luminescent biphosphine stabilized â€˜Cu₁₂S₆â€™ cluster molecules. Chemical Communications, 2014, 50, 11043.	2.2	46
52	Ionicâ€Radiusâ€Driven Selection of the Mainâ€Groupâ€Metal Cage for Intermetalloid Clusters [Ln@Pb_xBi_{14â^'x}]^{qâ^'} and [Ln@Pb_yBi_{13â^'y}]^{qâ^'} (x/q=7/4, 6/3;) Tj ETQq0 0 0 rgBT /Over	1.7	46
53	NMR Shielding Tensors and Chemical Shifts in Scalar-Relativistic Local Exact Two-Component Theory. Journal of Chemical Theory and Computation, 2019, 15, 1028-1043.	2.3	46
54	Off-Diagonal Self-Energy Terms and Partially Self-Consistency in GW Calculations for Single Molecules: Efficient Implementation and Quantitative Effects on Ionization Potentials. Journal of Chemical Theory and Computation, 2015, 11, 5152-5160.	2.3	42

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55	Structures and properties of neutral gallium clusters: A theoretical investigation. Journal of Chemical Physics, 2011, 135, 044314.	1.2	41
56	Atom distributions in binary atom clusters: A perturbational approach and its validation in a case study. Journal of Chemical Physics, 2004, 121, 10380-10384.	1.2	40
57	A Square As4 and a Prismatic As6 Structure as Complex Ligands. Chemistry - A European Journal, 1997, 3, 1494-1498.	1.7	39
58	Structures of small bismuth cluster cations. Journal of Chemical Physics, 2012, 136, 154309.	1.2	39
59	An NHCâ€“phosphinidenyl as a synthon for new group 13/15 compounds. Chemical Communications, 2017, 53, 7620-7623.	2.2	39
60	Phosphorescence lifetimes of organic light-emitting diodes from two-component time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 224302.	1.2	38
61	Silver Aggregation Caused by Stanna-closo-dodecaborate Coordination:Â Syntheses, Solid-State Structures and Theoretical Studies. Inorganic Chemistry, 2007, 46, 6775-6784.	1.9	37
62	Quantum chemical treatments of metal clusters. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 1245-1263.	1.6	37
63	[V@Ge₈As₄]^{3â^'} and [Nb@Ge₈As₆]^{3â^'}: encapsulation of electron-poor transition metal atoms. Chemical Communications, 2015, 51, 3866-3869.	2.2	37
64	Efficient two-component self-consistent field procedures and gradients: implementation in TURBOMOLE and application to. Molecular Physics, 2013, 111, 2617-2624.	0.8	36
65	Lowâ€Valent Groupâ€...14 Phosphinidenide Complexes [({SIDipp}P)₂M] Exhibit Pâ€“M pï€â€“pï€ Interaction (M=Ge, Sn, Pb). Chemistry - A European Journal, 2020, 26, 192-197.	1.7	36
66	Segmented Contracted Error-Consistent Basis Sets of Quadruple-Î¶ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. Journal of Chemical Theory and Computation, 2020, 16, 5658-5674.	2.3	36
67	(Ge₂P₂)^{2â^'}: a binary analogue of P₄as a precursor to the ternary cluster anion [Cd₃(Ge₃P)₃]^{3â^'}. Chemical Communications, 2018, 54, 1421-1424.	2.2	35
68	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
69	Ab initio treatment of (H2O)2- and (H2O)6-. Physical Chemistry Chemical Physics, 1999, 1, 4537-4540.	1.3	33
70	Title is missing!. Angewandte Chemie, 2003, 115, 1539-1543.	1.6	33
71	{Î¼â€PbSe}: A Heavy CO Homologue as an Unexpected Ligand. Angewandte Chemie - International Edition, 2015, 54, 11283-11288.	7.2	33
72	[Co@Sn₆Sb₆]^{3â^'}: An Offâ€Center Endohedral 12â€Vertex Cluster. Angewandte Chemie - International Edition, 2018, 57, 15359-15363.	7.2	33

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73	Extending DFT-based genetic algorithms by atom-to-place re-assignment via perturbation theory: A systematic and unbiased approach to structures of mixed-metallic clusters. Journal of Chemical Physics, 2014, 141, 134103.	1.2	31
74	[{Ag(tBuNH2)2}4][{Ag(tBuNH2)(tBuN=CHCH3)}2][Ag12(CF3CO2)14]: A Compound with an Ag128+ Cluster Core. Angewandte Chemie - International Edition, 2000, 39, 3925-3929.	7.2	30
75	Zinc Chalcogenolate Complexes as Precursors to ZnE and Mn/ZnE (E = S, Se) Clusters. Inorganic Chemistry, 2012, 51, 2747-2756.	1.9	30
76	Luminescence in Phosphine-Stabilized Copper Chalcogenide Cluster Moleculesâ€"A Comparative Study. Inorganic Chemistry, 2015, 54, 9413-9422.	1.9	29
77	Electronic structure and bonding in endohedral Zintl clusters. Chemical Society Reviews, 2022, 51, 628-649.	18.7	29
78	Stepwise Synthesis and Coordination Compound of an Inorganic Cryptand. Angewandte Chemie - International Edition, 2007, 46, 4775-4779.	7.2	28
79	Stabilizing a metalloid {Zn12} unit within a polymetallide environment in [K2Zn20Bi16]6â^'. Nature Communications, 2020, 11, 5122.	5.8	27
80	Atom Exchange Versus Reconstruction: (Ge_xAs_{4â^'x})^{xâ^'} (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au₆(Ge₃As)(Ge₂As₂)₃]^{3â^'}. Angewandte Chemie - International Edition, 2020, 59, 16638-16643.	7.2	27
81	NMR Indirect Spinâ€"Spin Coupling Constants in a Modern Quasi-Relativistic Density Functional Framework. Journal of Chemical Theory and Computation, 2021, 17, 3974-3994.	2.3	27
82	Influence of vibrations on electron transport through nanoscale contacts. Physica Status Solidi (B): Basic Research, 2013, 250, 2468-2480.	0.7	26
83	Simple but effective: thermally stable Cuâ€"ESiMe₃via NHC ligation. Chemical Communications, 2015, 51, 8361-8364.	2.2	26
84	[Hg 4 Te 8 (Te 2) 4] 8â^' : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. Angewandte Chemie - International Edition, 2018, 57, 8770-8774.	7.2	26
85	Synthese, Kristallstrukturen und quantenchemische Untersuchung von Verbindungen mit leiterartigem Al4P4- und hexagonal prismatischem Al6P6-GrundgerÃ¼st. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2002, 628, 389-393.	0.6	25
86	1â€Đâ€Tin(II) Phenylchalcogenolato Complexes _{â^ž}¹[Sn(EPh)₂] (E = S, Se,) Tj ETQq0 0 0 rgBT /O Inorganic Chemistry, 2010, 2010, 410-418.	1.0	25
87	The Identity of â€œTernaryâ€•A/Tl/Pb or K/Tl/Bi Solid Mixtures and Binary Zintl Anions Isolated From Their Solutions. Chemistry - A European Journal, 2018, 24, 12022-12030.	1.7	25
88	Atom-Type Assignment in Molecules and Clusters by Perturbation Theoryâ€"A Complement to X-ray Structure Analysis. Chemistry - A European Journal, 2005, 11, 3559-3564.	1.7	24
89	Vibrational circular dichroism spectra for large molecules and molecules with heavy elements. Journal of Chemical Physics, 2017, 146, 054102.	1.2	24
90	Phosphorescence Energies of Organic Lightâ€Emitting Diodes from Spinâ€Flip Tammâ€"Dancoff Approximation Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2011, 12, 3331-3336.	1.0	22

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91	Electron Paramagnetic Resonance and Density-Functional Theory Studies of Cu(II)-bis(oxamato) Complexes. Inorganic Chemistry, 2008, 47, 6633-6644.	1.9	21
92	One-Electron Energies from the Two-Component GW Method. Journal of Chemical Theory and Computation, 2015, 11, 969-979.	2.3	21
93	Introduction of plumbole to f-element chemistry. Chemical Science, 2022, 13, 945-954.	3.7	21
94	Bistrimethylsilylamide Transition-Metal Complexes as Starting Reagents in the Synthesis of Ternary Cdâ^'Mnâ^'Se Cluster Complexes. Inorganic Chemistry, 2010, 49, 7331-7339.	1.9	20
95	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. Journal of Physical Chemistry C, 2019, 123, 15354-15365.	1.5	20
96	Tuning the Metal/Chalcogen Composition in Copper(I)â€“Chalcogenide Clusters with Cyclic (Alkyl)(amino)carbene Ligands. Inorganic Chemistry, 2019, 58, 3338-3348.	1.9	20
97	Enhancement of and interference among higher order multipole transitions in molecules near a plasmonic nanoantenna. Nature Communications, 2019, 10, 5775.	5.8	19
98	Syntheses of the 47 Electron Clusters [(Cp*Fe)3(Î¼3-X)2] (X = S, Se) and the First Fe/Sn/Se Heterocubane Cluster [(Cp*Fe)3(SnCl3)(Î¼3-Se)4]·DME by the Use of Chalcogenostannate Salts. Inorganic Chemistry, 2004, 43, 4595-4603.	1.9	18
99	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. Physical Chemistry Chemical Physics, 2017, 19, 12794-12803.	1.3	18
100	Highly Soluble Supertetrahedra upon Selective Partial Butylation of Chalcogenido Metalate Clusters in Ionic Liquids. Angewandte Chemie - International Edition, 2021, 60, 17622-17628.	7.2	18
101	Synthesis and Reactivity of NHC€Stabilized Iron(II)â€“Mesityl Complexes. European Journal of Inorganic Chemistry, 2017, 2017, 2600-2616.	1.0	17
102	Not Non-Coordinating at All: Coordination Compounds of the Cyclodimethylsiloxanes D_n (D = Me₂SiO; n = 6, 7) and Group 2 Metal Cations. Inorganic Chemistry, 2019, 58, 15417-15422.	1.9	17
103	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
104	The Arachnoâ€Zintl Ion (Sn₅Sb₃)^{3â^'} and the Effects of Element Composition on the Structures of Isoelectronic Clusters: Another Facet of the Pseudoâ€Element Concept. Angewandte Chemie - International Edition, 2020, 59, 14251-14255.	7.2	17
105	Paramagnetic NMR Shielding Tensors and Ring Currents: Efficient Implementation and Application to Heavy Element Compounds. Journal of Physical Chemistry A, 2021, 125, 9707-9723.	1.1	17
106	Two-component hybrid time-dependent density functional theory within the Tamm-Dancoff approximation. Journal of Chemical Physics, 2015, 142, 034116.	1.2	16
107	Bis(6â€methyleneâ€2,2â€²â€bipyridine)phenylphosphineâ€”A Flexible Ligand for the Construction of Trinuclear Coinageâ€Metal Complexes. Chemistry - A European Journal, 2017, 23, 12198-12209.	1.7	16
108	Coinage Metal Complexes of Bisâ€Alkynylâ€Functionalized Nâ€Heterocyclic Carbenes: Reactivity, Photophysical Properties, and Quantum Chemical Investigations. Chemistry - A European Journal, 2017, 23, 1591-1603.	1.7	16

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109	Metalâ€Free Nâ^'H Bond Activation by Phosphaâ€Wittig Reagents**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	16
110	Observation and Interpretation of Structural Variety in Alkaline Earth Metal Derivatives of Diphosphanyldisiloxane. European Journal of Inorganic Chemistry, 2010, 2010, 258-265.	1.0	15
111	Probing the Influence of Size and Composition on the Photoelectron Spectra of Cadmium Chalcogenide Cluster Dianions. Journal of Physical Chemistry C, 2012, 116, 13800-13809.	1.5	15
112	[(Pb6I8){Mn(CO)5}6]2â€“: An Octahedral (M6X8)-like Cluster with Inverted Bonding. Inorganic Chemistry, 2015, 54, 3989-3994.	1.9	15
113	{[CuSn5Sb3]2â^'}2: Ein Dimer inhomogener Superatome. Angewandte Chemie, 2016, 128, 11950-11955.	1.6	15
114	Unique Manganese Phosphorus Complex with a Mn₅P₇ Core: Synthesis, Molecular Structure, and Magnetic Properties. Inorganic Chemistry, 2008, 47, 1460-1464.	1.9	14
115	Partial double bond character in chalcogen compounds of stanna-closo-dodecaborate. Dalton Transactions, 2009, , 1055-1062.	1.6	14
116	Chalcogen chemistry of group(iv) closo-dodecaborates, synthesis, theory and coordination chemistry. Dalton Transactions, 2010, 39, 7504.	1.6	14
117	Role of oxygen in the determination of oxide forming elements by electrothermal atomic absorption spectrometry Part 3. Effect of oxygen on the reactions of tin in uncoated, pyrolytically coated and zirconium carbide coated graphite tube atomizers. Spectrochimica Acta, Part B: Atomic Spectroscopy, 1996, 51, 1133-1137.	1.5	13
118	Synthesis, Structures and Theoretical Investigation of [Cu4(P2S6)(PPh3)4], [Cu6(P2S6)Cl2(PPh3)6], and [Au4(P2S6)(PPh3)4]. Chemistry - A European Journal, 2000, 6, 545-551.	1.7	13
119	Coherent transport through a molecular wire: DFT calculation. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 18, 255-257.	1.3	13
120	[Co@Sn 6 Sb 6] 3â^' : Ein endohedraler 12â€Atomâ€Cluster mit einem nichtâ€zentrierten inneren Atom. Angewandte Chemie, 2018, 130, 15585-15589.	1.6	13
121	Transitionâ€Metalâ€Induced Rearrangement of [(PhSn) 4 S 6] Towards Ternary Cu I /Sn/S or Cu II /Sn/S Clusters. Chemistry - A European Journal, 2019, 25, 2486-2490.	1.7	13
122	Optical properties of trinuclear metal chalcogenolate complexes â€“ room temperature NIR fluorescence in [Cu₂Ti(SPh)₆(PPh₃)₂]. Dalton Transactions, 2017, 46, 1502-1509.	1.6	12
123	Lowâ€Valent Groupâ€...14 NHCâ€Stabilized Phosphinidenide ate Complexes and NHCâ€Stabilized K/Pâ€Clusters. Chemistry - A European Journal, 2019, 25, 4914-4919.	1.7	12
124	Jahnâ€“Teller Distortion Versus Spinâ€“Orbit Splitting: Symmetry of Small Heavy-Metal Atom Clusters. Journal of Cluster Science, 2011, 22, 355-363.	1.7	11
125	Synthesis and Optical Properties of [Cu₆E₆(SnPh)₂(PPh₂Et)₆] (E = S, Se, Te) Cluster Molecules. Inorganic Chemistry, 2017, 56, 9330-9336.	1.9	11
126	Size Matters: From Twoâ€Dimensional Au^Iâ€“Tl^I Metallopolymers to Molecular Complexes by Simple Variation of the Steric Demand. Chemistry - A European Journal, 2019, 25, 3799-3808.	1.7	11

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127	Synthesis and Reactivity of Bis(silylene)â€Coordinated Calcium and Divalent Lanthanide Complexes. Chemistry - A European Journal, 2020, 26, 14888-14895.	1.7	11
128	The Archetypal Homoleptic Lanthanide Quadrupleâ€Deckerâ€"Synthesis, Mechanistic Studies, and Quantum Chemical Investigations. Angewandte Chemie - International Edition, 2021, 60, 24493-24499.	7.2	11
129	Magnetic and Optical Properties of Cu(II)â^'Bis(oxamato) Complexes:â€‰ Combined Quantum Chemical Density Functional Theory and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2008, 112, 5585-5593.	1.2	10
130	Enhancing Electrochemiluminescence of Chalcogenide Clusters by Means of Mn Replacement. Electrochimica Acta, 2016, 210, 79-86.	2.6	10
131	The chemical space of PbNâ^'nBin and (PbNâ^'nBin)+: A systematic study for N = 3â€"13. Journal of Chemical Physics, 2017, 146, 034304.	1.2	10
132	Construction of Inorganic Crown Ethers by sâ€Blockâ€Metalâ€Templated Siâ^'O Bond Activation. Angewandte Chemie - International Edition, 2021, 60, 10393-10401.	7.2	10
133	Tetrahedral [Sb(AuMe)₄]^{3â^'}Occurring in Multimetallic Cluster Syntheses: About the Structureâ€Directing Role of Methyl Groups. Angewandte Chemie - International Edition, 2021, 60, 25042-25047.	7.2	10
134	Synthesis of a Molecule with Five Different Adjacent Pnictogens. Chemistry - A European Journal, 2020, 26, 8536-8540.	1.7	10
135	Spin density distribution in oxamato-type transition metal complexes. Polyhedron, 2007, 26, 1773-1775.	1.0	9
136	Coordination and Oligomerisation of the Siloxanephosphane Cage Compound [P₂{(SiMe₂)₂O}₃]. Chemistry - A European Journal, 2009, 15, 9642-9646.	1.7	9
137	Neutral and cationic main group element cages of germanium(ii) with pyrazolyl ligands: solid state structures, DFT calculations and advanced solution NMR investigations. Dalton Transactions, 2009, , 5335.	1.6	9
138	Acceleration of selfâ€consistentâ€field convergence by combining conventional diagonalization and a diagonalizationâ€free procedure. Journal of Computational Chemistry, 2011, 32, 3129-3134.	1.5	9
139	[Hg 4 Te 8 (Te 2) 4] 8â^' : ein Schwermetallâ€Porphyrinoid in einer lamellaren Struktur. Angewandte Chemie, 2018, 130, 8906-8910.	1.6	9
140	Î· 3 â€Coordination and Functionalization of the 2â€Phosphaethynthiolate Anion at Lanthanum(III)**. Angewandte Chemie - International Edition, 2021, 60, 9534-9539.	7.2	9
141	NONâ€Ligated N â€Heterocyclic Tetrylenes. European Journal of Inorganic Chemistry, 2021, 2021, 3591-3600.	1.0	9
142	A Planar Fiveâ€Membered Aromatic Ring Stabilized by Only Two Ï€â€Electrons. Angewandte Chemie - International Edition, 2022, 61, .	7.2	8
143	[M@Sn_{14â€"x}Sb_x]^{qâ^'} (M = La, Ce, or U; x) Tj ETQq1 1 0.784314 rg Clusters. Inorganic Chemistry, 2023, 62, 1885-1890.	1.9	8
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