Florian Weigend

List of Publications by Citations

172 papers	35,167 citations	44 h-index	187 g-index
194 ext. papers	41,005 ext. citations	6.1 avg, IF	7.92 L-index

#	Paper	IF	Citations
172	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, 3297-305	3.6	14310
171	Accurate Coulomb-fitting basis sets for H to Rn. *Physical Chemistry Chemical Physics*, **2006**, 8, 1057-65	3.6	3695
170	Auxiliary basis sets for main row atoms and transition metals and their use to approximate Coulomb potentials. *Theoretical Chemistry Accounts*, **1997**, 97, 119-124	1.9	2788
169	RI-MP2: optimized auxiliary basis sets and demonstration of efficiency. *Chemical Physics Letters*, **1998**, 294, 143-152	2.5	2175
168	Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. *Journal of Chemical Physics*, **2002**, 116, 3175-3183	3.9	1456
167	RI-MP2: first derivatives and global consistency. *Theoretical Chemistry Accounts*, **1997**, 97, 331-340	1.9	1229
166	CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. *Journal of Chemical Physics*, **2000**, 113, 5154	3.9	1207
165	A fully direct RI-HF algorithm: Implementation, optimised auxiliary basis sets, demonstration of accuracy and efficiency. *Physical Chemistry Chemical Physics*, **2002**, 4, 4285-4291	3.6	1005
164	Gaussian basis sets of quadruple zeta valence quality for atoms H-Kr. *Journal of Chemical Physics*, **2003**, 119, 12753-12762	3.9	784
163	Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100	7.9	710
162	Hartree-Fock exchange fitting basis sets for H to Rn. *Journal of Computational Chemistry*, **2008**, 29, 167-75	3.5	436
161	A single-molecule diode. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 8815-20	11.5	402
160	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107	3.9	255
159	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
158	Conductance of molecular wires and transport calculations based on density-functional theory. *Physical Review B*, **2004**, 69,	3.3	176
157	The GW-Method for Quantum Chemistry Applications: Theory and Implementation. *Journal of Chemical Theory and Computation*, **2013**, 9, 232-46	6.4	174
156	Electronic transport through single conjugated molecules. *Chemical Physics*, **2002**, 281, 113-125	2.3	154

155	Approximated electron repulsion integrals: Cholesky decomposition versus resolution of the identity methods. *Journal of Chemical Physics*, **2009**, 130, 164106	3.9	144
154	Segmented contracted basis sets for one- and two-component Dirac-Fock effective core potentials. *Journal of Chemical Physics*, **2010**, 133, 174102	3.9	134
153	Slow magnetic relaxation in trigonal-planar mononuclear Fe(II) and Co(II) bis(trimethylsilyl)amido complexes--a comparative study. *Inorganic Chemistry*, **2014**, 53, 1962-74	5.1	128
152	Self-consistent treatment of spin-orbit interactions with efficient Hartree-Fock and density functional methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 1748-56	3.6	125
151	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. *Journal of Chemical Physics*, **2013**, 138, 184105	3.9	121
150	Theoretical study on clusters of magnesium. *Physical Chemistry Chemical Physics*, **2001**, 3, 711-719	3.6	112
149	Superatomic Orbitals under Spin-Orbit Coupling. *Journal of Physical Chemistry Letters*, **2014**, 5, 3286-9	6.4	99
148	Binding energies of CO on gold cluster cations Au n + (n=1-65): a radiative association kinetics study. *Journal of Chemical Physics*, **2005**, 122, 104702	3.9	99
147	Ortho-chalcogenostannates as ligands: syntheses, crystal structures, electronic properties, and magnetism of novel compounds containing ternary anionic substructures [M4(mu4-Se)(SnSe4)4]10- (M=Mn, Zn, Cd, Hg), 3(infinity)[[Hg4(mu4-Se)(SnSe4)3]6-], or 1(infinity)[[HgSnSe4]2-]. *Chemistry - A European Journal*, **2004**, 10, 5147-57	4.8	94
146	Quasi-Particle Self-Consistent GW for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2528-41	6.4	90
145	Unusual syntheses, structures, and electronic properties of compounds containing ternary, T3-type supertetrahedral M/Sn/S anions [M5Sn(mu3-S)4(SnS4)4](10- (M = Zn, Co). *Inorganic Chemistry*, **2005**, 44, 5686-95	5.1	83
144	Quantum chemistry calculations for molecules coupled to reservoirs: formalism, implementation, and application to benzenedithiol. *Journal of Chemical Physics*, **2007**, 126, 174101	3.9	81
143	Doped semimetal clusters: ternary, intermetalloid anions [Ln@Sn7Bi7]4- and [Ln@Sn4Bi9]4- (Ln = La, Ce) with adjustable magnetic properties. *Journal of the American Chemical Society*, **2012**, 134, 1181-91	16.4	78
142	Understanding of multimetallic cluster growth. *Nature Communications*, **2016**, 7, 10480	17.4	76
141	Segmented Contracted Error-Consistent Basis Sets of Double- and Triple-ζ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3696-3705	6.4	74
140	Error-Balanced Segmented Contracted Basis Sets of Double-ζ to Quadruple-ζ Valence Quality for the Lanthanides. *Journal of Chemical Theory and Computation*, **2012**, 8, 4062-8	6.4	63
139	Main Group Metal-Actinide Magnetic Coupling and Structural Response Upon U(4+) Inclusion Into Bi, Tl/Bi, or Pb/Bi Cages. *Journal of the American Chemical Society*, **2016**, 138, 9033-6	16.4	57
138	Structural relaxation in charged metal surfaces and cluster ions. *Small*, **2006**, 2, 1497-503	11	56

137	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	3.9	55
136	Basis-set extensions for two-component spin-orbit treatments of heavy elements. *Physical Chemistry Chemical Physics*, **2006**, 8, 4862-5	3.6	54
135	Making practical use of the pseudo-element concept: an efficient way to ternary intermetalloid clusters by an isoelectronic Pb(-)-Bi combination. *Chemical Communications*, **2012**, 48, 11295-7	5.8	53
134	Binding energy and preferred adsorption sites of CO on gold and silver-gold cluster cations: adsorption kinetics and quantum chemical calculations. *Faraday Discussions*, **2008**, 138, 393-406; discussion 421-34	3.6	52
133	A N-Heterocyclic Carbene-Stabilized Coinage Metal-Chalcogenide Framework with Tunable Optical Properties. *Journal of the American Chemical Society*, **2017**, 139, 14045-14048	16.4	50
132	Seminumerical calculation of the Hartree-Fock exchange matrix: application to two-component procedures and efficient evaluation of local hybrid density functionals. *Journal of Computational Chemistry*, **2012**, 33, 810-6	3.5	47
131	Implementation of Two-Component Time-Dependent Density Functional Theory in TURBOMOLE. *Journal of Chemical Theory and Computation*, **2013**, 9, 5341-8	6.4	45
130	Gold-gold interaction--stannaborate [SnB11H11]2- coordination chemistry. *Angewandte Chemie - International Edition*, **2003**, 42, 1501-5	16.4	45
129	Red-luminescent biphosphine stabilized M□SM cluster molecules. *Chemical Communications*, **2014**, 50, 11043-5	5.8	44
128	Subtle impact of atomic ratio, charge and lewis basicity on structure selection and stability: the Zintl anion [(La@In2Bi11)(□Bi)2(La@In2Bi11)]6-. *Chemistry - A European Journal*, **2012**, 18, 13589-95	4.8	43
127	Unusual 14-electron fragments [Pd(□) -Bi3-x Pbx)]((x+1)-) as pseudo lead atoms in closo-[Pd@Pd2 Pb10 Bi6](4-). *Angewandte Chemie - International Edition*, **2013**, 52, 13544-8	16.4	43
126	Ionic-radius-driven selection of the main-group-metal cage for intermetalloid clusters [Ln@Pbx Bi14-x](q-) and [Ln@Pby Bi13-y](q-) (x/q=7/4, 6/3; y/q=4/4, 3/3). *Chemistry - A European Journal*, **2015**, 21, 386-94	4.8	38
125	{[CuSn5 Sb3](2-) }2 : A Dimer of Inhomogeneous Superatoms. *Angewandte Chemie - International Edition*, **2016**, 55, 11775-80	16.4	37
124	Atom distributions in binary atom clusters: a perturbational approach and its validation in a case study. *Journal of Chemical Physics*, **2004**, 121, 10380-4	3.9	37
123	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, 5152-60	6.4	36
122	Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. *Journal of Chemical Physics*, **2018**, 148, 104110	3.9	36
121	Structures and properties of neutral gallium clusters: a theoretical investigation. *Journal of Chemical Physics*, **2011**, 135, 044314	3.9	36
120	Phosphorescence lifetimes of organic light-emitting diodes from two-component time-dependent density functional theory. *Journal of Chemical Physics*, **2014**, 141, 224302	3.9	34

119	Quantum chemical treatments of metal clusters. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 1245-63	3	34
118	A Square As4 and a Prismatic As6 Structure as Complex Ligands. *Chemistry - A European Journal*, **1997**, 3, 1494-1498	4.8	34
117	[V@Ge8As4]3- and [Nb@Ge8As6]3-: encapsulation of electron-poor transition metal atoms. *Chemical Communications*, **2015**, 51, 3866-9	5.8	33
116	Silver aggregation caused by Stanna-closo-dodecaborate coordination: syntheses, solid-state structures and theoretical studies. *Inorganic Chemistry*, **2007**, 46, 6775-84	5.1	32
115	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	6.4	30
114	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	3.9	30
113	Structures of small bismuth cluster cations. *Journal of Chemical Physics*, **2012**, 136, 154309	3.9	29
112	Gold?Gold Interaction Stannaborate [SnB11H11]2 Coordination Chemistry. *Angewandte Chemie*, **2003**, 115, 1539-1543	3.6	29
111	An NHC-phosphinidenyl as a synthon for new group 13/15 compounds. *Chemical Communications*, **2017**, 53, 7620-7623	5.8	28
110	Efficient two-component self-consistent field procedures and gradients: implementation in TURBOMOLE and application to. *Molecular Physics*, **2013**, 111, 2617-2624	1.7	28
109	Ab initio treatment of (H2O)2- and (H2O)6-. *Physical Chemistry Chemical Physics*, **1999**, 1, 4537-4540	3.6	28
108	(GeP): a binary analogue of P as a precursor to the ternary cluster anion [Cd(GeP)]. *Chemical Communications*, **2018**, 54, 1421-1424	5.8	27
107	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	3.6	27
106	{PbSe}: a heavy CO homologue as an unexpected ligand. *Angewandte Chemie - International Edition*, **2015**, 54, 11283-8	16.4	27
105	NMR Shielding Tensors and Chemical Shifts in Scalar-Relativistic Local Exact Two-Component Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 1028-1043	6.4	27
104	Simple but effective: thermally stable Cu-ESiMe3via NHC ligation. *Chemical Communications*, **2015**, 51, 8361-4	5.8	26
103	Zinc chalcogenolate complexes as precursors to ZnE and Mn/ZnE (E = S, Se) clusters. *Inorganic Chemistry*, **2012**, 51, 2747-56	5.1	26
102	Ungewöhnliche 14-Elektronen-Fragmente [Pd(η3-Bi3Pbx)](x+1) als Pseudo-Bleiatome in closo-[Pd@Pd2Pb10Bi6]4 *Angewandte Chemie*, **2013**, 125, 13786-13790	3.6	26

101	[{Ag(tBuNH) }][{Ag(tBuNH)(tBuN=CHCH)}][Ag (CF CO)]: A Compound with an Ag Cluster Core. *Angewandte Chemie - International Edition*, **2000**, 39, 3925-3929	16.4	26
100	Luminescence in phosphine-stabilized copper chalcogenide cluster molecules--a comparative study. *Inorganic Chemistry*, **2015**, 54, 9413-22	5.1	25
99	Stepwise synthesis and coordination compound of an inorganic cryptand. *Angewandte Chemie - International Edition*, **2007**, 46, 4775-9	16.4	25
98	[Co@Sn Sb] : An Off-Center Endohedral 12-Vertex Cluster. *Angewandte Chemie - International Edition*, **2018**, 57, 15359-15363	16.4	25
97	Synthese, Kristallstrukturen und quantenchemische Untersuchung von Verbindungen mit leiterartigem Al4P4- und hexagonal prismatischem Al6P6-Grundgerüst. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2002**, 628, 389-393	1.3	24
96	1-D-Tin(II) Phenylchalcogenolato Complexes [Sn(EPh)2] (E = S, Se, Te) Synthesis, Structures, Quantum Chemical Studies and Thermal Behaviour. *European Journal of Inorganic Chemistry*, **2010**, 2010, 410-418	2.3	23
95	Atom-type assignment in molecules and clusters by perturbation theory-A complement to X-ray structure analysis. *Chemistry - A European Journal*, **2005**, 11, 3559-64	4.8	23
94	Substantial Aromaticity in the anionic heavy-metal cluster [Th@Bi]. *Nature Chemistry*, **2021**, 13, 149-155	17.6	22
93	Influence of vibrations on electron transport through nanoscale contacts. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2468-2480	1.3	21
92	Phosphorescence energies of organic light-emitting diodes from spin-flip Tamm-Dancoff approximation time-dependent density functional theory. *ChemPhysChem*, **2011**, 12, 3331-6	3.2	21
91	Electron paramagnetic resonance and density-functional theory studies of Cu(II)-bis(oxamato) complexes. *Inorganic Chemistry*, **2008**, 47, 6633-44	5.1	21
90	Bistrimethylsilylamide transition-metal complexes as starting reagents in the synthesis of ternary Cd-Mn-Se cluster complexes. *Inorganic Chemistry*, **2010**, 49, 7331-9	5.1	20
89	The Identity of "Ternary" 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	4.8	19
88	An Efficient Coupled-Perturbed Kohn-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	6.4	19
87	Atom Exchange Versus Reconstruction: (Ge As) (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au (Ge As)(Ge As)]. *Angewandte Chemie - International Edition*, **2020**, 59, 16638-16643	16.4	17
86	[Hg Te (Te)] : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. *Angewandte Chemie - International Edition*, **2018**, 57, 8770-8774	16.4	17
85	Syntheses of the 47 electron clusters [(Cp*Fe)3(mu3-X)2] (X = S, Se) and the First Fe/Sn/Se Heterocubane Cluster [(CpFe)3(SnCl3)(mu3-Se)4] x DME by the use of chalcogenostannate salts. *Inorganic Chemistry*, **2004**, 43, 4595-603	5.1	17
84	Low-Valent Group 14 Phosphinidenide Complexes [({SIDipp}P) M] Exhibit P-M pπ-pπ Interaction (M=Ge, Sn, Pb). *Chemistry - A European Journal*, **2020**, 26, 192-197	4.8	17

83	One-Electron Energies from the Two-Component GW Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 969-79	6.4	16
82	Vibrational circular dichroism spectra for large molecules and molecules with heavy elements. *Journal of Chemical Physics*, **2017**, 146, 054102	3.9	15
81	Ein anorganischer Cryptand: schrittweise Synthese und Koordination von Li+-Ionen. *Angewandte Chemie*, **2007**, 119, 4859-4863	3.6	15
80	Stabilizing a metalloid {Zn} unit within a polymetallide environment in [KZnBi]. *Nature Communications*, **2020**, 11, 5122	17.4	15
79	Bis(6-methylene-2,2′-bipyridine)phenylphosphine-A Flexible Ligand for the Construction of Trinuclear Coinage-Metal Complexes. *Chemistry - A European Journal*, **2017**, 23, 12198-12209	4.8	14
78	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. *Physical Chemistry Chemical Physics*, **2017**, 19, 12794-12803	3.6	14
77	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	3.8	14
76	Chalcogen chemistry of group(IV) closo-dodecaborates, synthesis, theory and coordination chemistry. *Dalton Transactions*, **2010**, 39, 7504-12	4.3	14
75	Observation and Interpretation of Structural Variety in Alkaline Earth Metal Derivatives of Diphosphanyldisiloxane. *European Journal of Inorganic Chemistry*, **2010**, 2010, 258-265	2.3	14
74	Unique manganese phosphorus complex with a Mn5P7 core: synthesis, molecular structure, and magnetic properties. *Inorganic Chemistry*, **2008**, 47, 1460-4	5.1	14
73	{[CuSn5Sb3]2}2-: Ein Dimer inhomogener Superatome. *Angewandte Chemie*, **2016**, 128, 11950-11955	3.6	14
72	Tuning the Metal/Chalcogen Composition in Copper(I)-Chalcogenide Clusters with Cyclic (Alkyl)(amino)carbene Ligands. *Inorganic Chemistry*, **2019**, 58, 3338-3348	5.1	14
71	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. *Journal of Physical Chemistry C*, **2019**, 123, 15354-15365	3.8	13
70	[(Pb6I8){Mn(CO)5}6](2-): an octahedral (M6X8)-like cluster with inverted bonding. *Inorganic Chemistry*, **2015**, 54, 3989-94	5.1	13
69	Partial double bond character in chalcogen compounds of stanna-closo-dodecaborate. *Dalton Transactions*, **2009**, 1055-62	4.3	13
68	Theoretical Investigation of Binary and Ternary Metal Clusters derived from [Y10M]n+ Zintl Ions. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2002**, 628, 2478-2482	1.3	13
67	Segmented Contracted Error-Consistent Basis Sets of Quadruple-ζ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 5658-5674	6.4	13
66	Enhancement of and interference among higher order multipole transitions in molecules near a plasmonic nanoantenna. *Nature Communications*, **2019**, 10, 5775	17.4	13

65	Transition-Metal-Induced Rearrangement of [(PhSn) S] Towards Ternary Cu /Sn/S or Cu /Sn/S Clusters. *Chemistry - A European Journal*, **2019**, 25, 2486-2490	4.8	13
64	Synthesis and Reactivity of NHC-Stabilized Iron(II) Mesityl Complexes. *European Journal of Inorganic Chemistry*, **2017**, 2017, 2600-2616	2.3	12
63	Two-component hybrid time-dependent density functional theory within the Tamm-Dancoff approximation. *Journal of Chemical Physics*, **2015**, 142, 034116	3.9	12
62	Not Non-Coordinating at All: Coordination Compounds of the Cyclodimethylsiloxanes D (D = MeSiO; = 6, 7) and Group 2 Metal Cations. *Inorganic Chemistry*, **2019**, 58, 15417-15422	5.1	12
61	Coinage Metal Complexes of Bis-Alkynyl-Functionalized N-Heterocyclic Carbenes: Reactivity, Photophysical Properties, and Quantum Chemical Investigations. *Chemistry - A European Journal*, **2017**, 23, 1591-1603	4.8	12
60	[Co@Sn6Sb6]3 Ein endohedraler 12-Atom-Cluster mit einem nicht-zentrierten inneren Atom. *Angewandte Chemie*, **2018**, 130, 15585-15589	3.6	12
59	PbSe: ein schweres CO-Homolog als ungewnlicher Ligand. *Angewandte Chemie*, **2015**, 127, 11437-11442	3.6	11
58	Coherent transport through a molecular wire: DFT calculation. *Physica E: Low-Dimensional Systems and Nanostructures*, **2003**, 18, 255-257	3	11
57	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	3.1	11
56	Optical properties of trinuclear metal chalcogenolate complexes - room temperature NIR fluorescence in [CuTi(SPh)(PPh)]. *Dalton Transactions*, **2017**, 46, 1502-1509	4.3	10
55	Enhancing Electrochemiluminescence of Chalcogenide Clusters by Means of Mn Replacement. *Electrochimica Acta*, **2016**, 210, 79-86	6.7	10
54	Synthesis and Optical Properties of [CuE(SnPh)(PPhEt)] (E = S, Se, Te) Cluster Molecules. *Inorganic Chemistry*, **2017**, 56, 9330-9336	5.1	10
53	Jahn Teller Distortion Versus Spin Orbit Splitting: Symmetry of Small Heavy-Metal Atom Clusters. *Journal of Cluster Science*, **2011**, 22, 355-363	3	10
52	Magnetic and optical properties of Cu(II)-bis(oxamato) complexes: combined quantum chemical density functional theory and vibrational spectroscopy studies. *Journal of Physical Chemistry B*, **2008**, 112, 5585-93	3.4	10
51	Nuclear Spin-Spin Couplings: Efficient Evaluation of Exact Exchange and Extension to Local Hybrid Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 8529-8539	2.8	10
50	NMR Indirect Spin-Spin Coupling Constants in a Modern Quasi-Relativistic Density Functional Framework. *Journal of Chemical Theory and Computation*, **2021**, 17, 3974-3994	6.4	10
49	The Arachno-Zintl Ion (Sn Sb) and the Effects of Element Composition on the Structures of Isoelectronic Clusters: Another Facet of the Pseudo-Element Concept. *Angewandte Chemie - International Edition*, **2020**, 59, 14251-14255	16.4	10
48	Coordination and oligomerisation of the siloxanephosphane cage compound [P(2){(SiMe(2))(2)O}(3)]. *Chemistry - A European Journal*, **2009**, 15, 9642-6	4.8	9

47	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**, 5335-47	4.2	9
46	Synthesis, structures and theoretical investigation of. *Chemistry - A European Journal*, **2000**, 6, 545-51	4.8	9
45	[{Ag(tBuNH2)2}4][{Ag(tBuNH2)(tBuN=CHCH3)}2][Ag12(CF3CO2)14] □eine Verbindung mit einem Ag128+-Clusterkern. *Angewandte Chemie*, **2000**, 112, 4085-4089	3.6	9
44	Size Matters: From Two-Dimensional Au -Tl Metallopolymers to Molecular Complexes by Simple Variation of the Steric Demand. *Chemistry - A European Journal*, **2019**, 25, 3799-3808	4.8	8
43	Spin density distribution in oxamato-type transition metal complexes. *Polyhedron*, **2007**, 26, 1773-1775	2.7	8
42	Synthesis of a Molecule with Five Different Adjacent Pnictogens. *Chemistry - A European Journal*, **2020**, 26, 8536-8540	4.8	8
41	Low-Valent Group 14 NHC-Stabilized Phosphinidenide ate Complexes and NHC-Stabilized K/P-Clusters. *Chemistry - A European Journal*, **2019**, 25, 4914-4919	4.8	7
40	[Hg4Te8(Te2)4]8□ein Schwermetall-Porphyrinoid in einer lamellaren Struktur. *Angewandte Chemie* , **2018**, 130, 8906-8910	3.6	7
39	The chemical space of PbBi and (PbBi): A systematic study for N = 3-13. *Journal of Chemical Physics*, **2017**, 146, 034304	3.9	6
38	A Controlled Route to a Luminescent 3 d -5 d Sulfido Cluster Containing Unique AuCu (□S) Motifs. *Chemistry - A European Journal*, **2016**, 22, 18378-18382	4.8	6
37	Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure. *Journal of Computational Chemistry*, **2011**, 32, 3129-34	3.5	6
36	Synthesis and Reactivity of Bis(silylene)-Coordinated Calcium and Divalent Lanthanide Complexes. *Chemistry - A European Journal*, **2020**, 26, 14888-14895	4.8	6
35	□Coordination and Functionalization of the 2-Phosphaethynthiolate Anion at Lanthanum(III)*. *Angewandte Chemie - International Edition*, **2021**, 60, 9534-9539	16.4	6
34	A combined experimental and quantum chemical study on thallium(I) tris(pyrazolyl)methanide. *Polyhedron*, **2017**, 125, 74-79	2.7	5
33	Paramagnetic NMR Shielding Tensors and Ring Currents: Efficient Implementation and Application to Heavy Element Compounds. *Journal of Physical Chemistry A*, **2021**, 125, 9707-9723	2.8	5
32	The coordination behavior of 2,3-bis(diphenylphosphino)maleic-N-phenylimide towards copper, silver, gold and palladium. *Dalton Transactions*, **2019**, 48, 6863-6871	4.3	4
31	Electronic structure and bonding in endohedral Zintl clusters.. *Chemical Society Reviews*, **2021**,	58.5	4
30	Introduction of plumbole to f-element chemistry.. *Chemical Science*, **2022**, 13, 945-954	9.4	4

29	-Coordination and Functionalization of the 2-Phosphaethynthiolate Anion at Lanthanum(III)**. *Angewandte Chemie*, **2021**, 133, 9620-9625	3.6	4
28	The Arachno-Zintl Ion (Sn5Sb3)3 and the Effects of Element Composition on the Structures of Isoelectronic Clusters: Another Facet of the Pseudo-Element Concept. *Angewandte Chemie*, **2020**, 132, 14357-14361	3.6	3
27	How photoelectron spectroscopy and quantum chemical studies can help understanding the magnetic properties of molecules: an example from the class of Cu(II)-bis(oxamato) complexes. *Journal of Physical Chemistry B*, **2009**, 113, 10051-4	3.4	3
26	Preparation and luminescence properties of a M heterometallic coinage metal chalcogenide cluster. *Dalton Transactions*, **2020**, 49, 593-597	4.3	3
25	A Series of Homoleptic Linear Trimethylsilylchalcogenido Cuprates, Argentates and Aurates Cat[MeSiE-M-ESiMe] (M = Cu, Ag, Au; E = S, Se). *Inorganic Chemistry*, **2020**, 59, 17565-17572	5.1	3
24	Construction of Inorganic Crown Ethers by s-Block-Metal-Templated Si-O Bond Activation. *Angewandte Chemie - International Edition*, **2021**, 60, 10393-10401	16.4	3
23	Highly Soluble Supertetrahedra upon Selective Partial Butylation of Chalcogenido Metalate Clusters in Ionic Liquids. *Angewandte Chemie - International Edition*, **2021**, 60, 17622-17628	16.4	3
22	The Archetypal Homoleptic Lanthanide Quadruple-Decker-Synthesis, Mechanistic Studies, and Quantum Chemical Investigations. *Angewandte Chemie - International Edition*, **2021**, 60, 24493-24499	16.4	3
21	Error-Balanced Segmented Contracted Gaussian Basis Sets **2015**, 181-194		1
20	Using a Porphyrin Diacid Cation to Stabilize a Square-Pyramidal BiX (X = Br, Cl/Br) Unit. *Inorganic Chemistry*, **2021**, 60, 4352-4356	5.1	1
19	Tracing the Jahn-Teller Distortion of C60n in Isostructural Fullerides [M(NH3)7]C60 ? NH3, M=Ba, Sr, K. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2021**, 647, 1132-1138	1.3	1
18	Quantum Chemical Investigations of Clusters of Heavy Metal Atoms. *Structure and Bonding*, **2016**, 41-62	0.9	1
17	Photochemistry with Chlorine Trifluoride: Syntheses and Characterization of Difluorooxychloronium(V) Hexafluorido(non)metallates(V), [ClOF][MF] (M=V, Nb, Ta, Ru, Os, Ir, P, Sb). *Chemistry - A European Journal*, **2021**, 27, 2381-2392	4.8	1
16	Aufbau anorganischer Kronenether durch s-Block-Metall-templatgesteuerte Si-O-Bindungsaktivierung. *Angewandte Chemie*, **2021**, 133, 10481-10490	3.6	1
15	Structure and Reactivity of Alkaline Metal Bis(amido)diazadiarsetidinides. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2021**, 647, 1830-1839	1.3	1
14	Tetrahedral [Sb(AuMe)4]3 Occurring in Multimetallic Cluster Syntheses: About the Structure-Directing Role of Methyl Groups. *Angewandte Chemie*, **2021**, 133, 25246	3.6	1
13	Tetrahedral [Sb(AuMe)] Occurring in Multimetallic Cluster Syntheses: About the Structure-Directing Role of Methyl Groups. *Angewandte Chemie - International Edition*, **2021**, 60, 25042-25047	16.4	1
12	Reduction of rhenates(VII) with hydrogen chloride in alcohols: The structural aspects of the trans-tetrachloridomethoxidooxidorhenate(VI) products. *Inorganica Chimica Acta*, **2014**, 411, 26-29	2.7	0

List of Publications

11	Near-Infrared Luminescence in Trinuclear Mixed-Metal Chalcogenolate Complexes of the Types [MTi(EPh)(PPh)] (M = Cu, Ag; E = S, Se) and [Na(thf)][Ti(SPh)]. *Inorganic Chemistry*, **2021**, 60, 8936-8945	5.1	0
10	Highly Soluble Supertetrahedra upon Selective Partial Butylation of Chalcogenido Metalate Clusters in Ionic Liquids. *Angewandte Chemie*, **2021**, 133, 17763-17769	3.6	0
9	Reactions of ThX4 (X=F, Cl, Br, I) with Liquid Ammonia-Crystal Structures and a Theoretical Study of Ammine Thorium(IV) Halide Ammoniates. *European Journal of Inorganic Chemistry*, **2021**, 2021, 2787-2796	2.3	0
8	The Archetypal Homoleptic Lanthanide Quadruple-Decker: Synthesis, Mechanistic Studies, and Quantum Chemical Investigations. *Angewandte Chemie*, **2021**, 133, 24698	3.6	0
7	NON-Ligated N-Heterocyclic Tetrylenes. *European Journal of Inorganic Chemistry*, **2021**, 2021, 3591-3600	2.3	0
6	Synthesis, Crystal Structure and Bond Situation of [Co7Se7Cp3(CO)4] (Cp = Cyclopentadienyl). *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2009**, 635, 2288-2293	1.3	
5	Ab Initio Calculations of Clusters. *Lecture Notes in Physics*, **2005**, 205-219	0.8	
4	Atom Exchange Versus Reconstruction: (GexAs4−x)x− (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au6(Ge3As)(Ge2As2)3]3− *Angewandte Chemie*, **2020**, 132, 16781	3.6	
3	Rücktitelbild: Atom Exchange Versus Reconstruction: (GexAs4−x)x− (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au6(Ge3As)(Ge2As2)3]3− (Angew. Chem. 38/2020). *Angewandte Chemie*, **2020**, 132, 16948	3.6	
2	Planar Iron Hydride Nanoclusters: Combined Spectroscopic and Theoretical Insights into Structures and Building Principles. *ChemistryOpen*, **2021**, 10, 265-271	2.3	
1	Surprises in the Solvent-Induced Self-Ionization in the Uranium Tetrahalide UX (X = Cl, Br, I)/Ethyl Acetate System.. *ACS Omega*, **2022**, 7, 11995-12003	3.9	