

Filipp Furche

List of Publications by Citations

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140
papers

15,196
citations

57
h-index

123
g-index

155
ext. papers

16,666
ext. citations

6.9
avg, IF

6.99
L-index

#	Paper	IF	Citations
140	Adiabatic time-dependent density functional methods for excited state properties. <i>Journal of Chemical Physics</i> , 2002 , 117, 7433-7447	3.9	1777
139	Property-optimized gaussian basis sets for molecular response calculations. <i>Journal of Chemical Physics</i> , 2010 , 133, 134105	3.9	1040
138	Gaussian basis sets of quadruple zeta valence quality for atoms H-Rn. <i>Journal of Chemical Physics</i> , 2003 , 119, 12753-12762	3.9	784
137	Turbomole. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 91-100	7.9	710
136	An efficient implementation of second analytical derivatives for density functional methods. <i>Chemical Physics Letters</i> , 2002 , 362, 511-518	2.5	520
135	The structures of small gold cluster anions as determined by a combination of ion mobility measurements and density functional calculations. <i>Journal of Chemical Physics</i> , 2002 , 117, 6982-6990	3.9	498
134	The performance of semilocal and hybrid density functionals in 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006 , 124, 044103	3.9	488
133	Circular Dichroism of Helicenes Investigated by Time-Dependent Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2000 , 122, 1717-1724	16.4	431
132	Structures of small gold cluster cations (Au _n ⁺ , n. <i>Journal of Chemical Physics</i> , 2002 , 116, 4094-4101	3.9	422
131	Molecular tests of the random phase approximation to the exchange-correlation energy functional. <i>Physical Review B</i> , 2001 , 64,	3.3	360
130	On the density matrix based approach to time-dependent density functional response theory. <i>Journal of Chemical Physics</i> , 2001 , 114, 5982-5992	3.9	349
129	Nuclear second analytical derivative calculations using auxiliary basis set expansions. <i>Chemical Physics Letters</i> , 2004 , 384, 103-107	2.5	326
128	Electron correlation methods based on the random phase approximation. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	315
127	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020 , 152, 184107	3.9	255
126	2D-3D transition of gold cluster anions resolved. <i>Physical Review A</i> , 2008 , 77,	2.6	243
125	Completing the series of +2 ions for the lanthanide elements: synthesis of molecular complexes of Pr ²⁺ , Gd ²⁺ , Tb ²⁺ , and Lu ²⁺ . <i>Journal of the American Chemical Society</i> , 2013 , 135, 9857-68	16.4	234
124	Efficient characterization of stationary points on potential energy surfaces. <i>Journal of Chemical Physics</i> , 2002 , 117, 9535-9538	3.9	233

123	Photoinduced intramolecular charge transfer in 4-(dimethyl)aminobenzonitrile--a theoretical perspective. <i>Journal of the American Chemical Society</i> , 2004 , 126, 1277-84	16.4	230
122	Developing the random phase approximation into a practical post-Kohn-Sham correlation model. <i>Journal of Chemical Physics</i> , 2008 , 129, 114105	3.9	223
121	Fast computation of molecular random phase approximation correlation energies using resolution of the identity and imaginary frequency integration. <i>Journal of Chemical Physics</i> , 2010 , 132, 234114	3.9	190
120	Fluctuation-dissipation theorem density-functional theory. <i>Journal of Chemical Physics</i> , 2005 , 122, 164105	3.9	180
119	An improved method for density functional calculations of the frequency-dependent optical rotation. <i>Chemical Physics Letters</i> , 2002 , 361, 321-328	2.5	175
118	First-order nonadiabatic couplings from time-dependent hybrid density functional response theory: Consistent formalism, implementation, and performance. <i>Journal of Chemical Physics</i> , 2010 , 132, 044107	3.9	174
117	Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. <i>Theoretical and Computational Chemistry</i> , 2005 , 16, 93-128		169
116	Identification of the +2 oxidation state for uranium in a crystalline molecular complex, [K(2.2.2-cryptand)][(C ₅ H ₄ SiMe ₃) ₃ U]. <i>Journal of the American Chemical Society</i> , 2013 , 135, 13310-3	16.4	166
115	Expanding rare-earth oxidation state chemistry to molecular complexes of holmium(II) and erbium(II). <i>Journal of the American Chemical Society</i> , 2012 , 134, 8420-3	16.4	149
114	Structural, spectroscopic, and theoretical comparison of traditional vs recently discovered Ln(2+) ions in the [K(2.2.2-cryptand)][(C ₅ H ₄ SiMe ₃) ₃ Ln] complexes: the variable nature of Dy(2+) and Nd(2+). <i>Journal of the American Chemical Society</i> , 2015 , 137, 369-82	16.4	146
113	Assessing Excited State Methods by Adiabatic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2376-86	6.4	146
112	Au ₃₄ : a chiral gold cluster?. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 2944-8	16.4	127
111	A Parameter-Free Density Functional That Works for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 983-989	6.4	124
110	Analytical time-dependent density functional derivative methods within the RI-J approximation, an approach to excited states of large molecules. <i>Journal of Chemical Physics</i> , 2005 , 122, 064105	3.9	119
109	Excited States from Time-Dependent Density Functional Theory. <i>Reviews in Computational Chemistry</i> , 2009 , 91-165		115
108	Ab initio non-adiabatic molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 18336-48	3.6	113
107	Synthesis and Magnetism of Neutral, Linear Metallocene Complexes of Terbium(II) and Dysprosium(II). <i>Journal of the American Chemical Society</i> , 2019 , 141, 12967-12973	16.4	109
106	Isolation of dysprosium and yttrium complexes of a three-electron reduction product in the activation of dinitrogen, the (N ₂) ³⁻ radical. <i>Journal of the American Chemical Society</i> , 2009 , 131, 11195-202	16.4	99

105	Synthesis, structure, and reactivity of crystalline molecular complexes of the $\{[\text{CH}(\text{SiMe})]\text{Th}\}$ anion containing thorium in the formal +2 oxidation state. <i>Chemical Science</i> , 2015 , 6, 517-521	9.4	89
104	Identification of the Formal +2 Oxidation State of Plutonium: Synthesis and Characterization of $\{\text{Pu}[\text{CH}(\text{SiMe})]\}$. <i>Journal of the American Chemical Society</i> , 2017 , 139, 3970-3973	16.4	87
103	Circular dichroism: electronic. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012 , 2, 150-166	7.9	81
102	Basis set convergence of molecular correlation energy differences within the random phase approximation. <i>Journal of Chemical Physics</i> , 2012 , 136, 084105	3.9	81
101	Random-Phase Approximation Methods. <i>Annual Review of Physical Chemistry</i> , 2017 , 68, 421-445	15.7	80
100	Communication: Random phase approximation renormalized many-body perturbation theory. <i>Journal of Chemical Physics</i> , 2013 , 139, 171103	3.9	78
99	Harnessing the meta-generalized gradient approximation for time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 164105	3.9	75
98	Facile bismuth-oxygen bond cleavage, C-H activation, and formation of a monodentate carbon-bound oxyaryl dianion, $(\text{C}(\text{H})(\text{t})\text{Bu})\text{B}, 5\text{-O-4})$. <i>Journal of the American Chemical Society</i> , 2011 , 133, 5244-7	16.4	74
97	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20986-98	3.6	71
96	Lagrangian approach to molecular vibrational Raman intensities using time-dependent hybrid density functional theory. <i>Journal of Chemical Physics</i> , 2007 , 126, 201104	3.9	71
95	Comment on Assessment of exchange correlation functionals [A.J. Cohen, N.C. Handy, Chem. Phys. Lett. 316 (2000) 160-166]. <i>Chemical Physics Letters</i> , 2000 , 325, 317-321	2.5	70
94	Synthesis, structure, and magnetism of an f element nitrosyl complex, $(\text{C}_5\text{Me}_4\text{H})_3\text{UNO}$. <i>Journal of the American Chemical Society</i> , 2012 , 134, 1243-9	16.4	68
93	Electronic photodissociation spectroscopy of $\text{Au}n - x \text{Xe}$ ($n = 7-11$) versus time-dependent density functional theory prediction. <i>Journal of Chemical Physics</i> , 2004 , 121, 4619-27	3.9	66
92	Synthesis of the $(\text{N}_2)_3^-$ radical from Y_2^+ and its protonolysis reactivity to form $(\text{N}_2\text{H}_2)_2^-$ via the $\text{Y}[\text{N}(\text{SiMe}_3)_2]_3/\text{KC}_8$ reduction system. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3784-7	16.4	63
91	Fullerene C80: Are there still more isomers?. <i>Journal of Chemical Physics</i> , 2001 , 114, 10362-10367	3.9	63
90	Solution Synthesis, Structure, and CO Reduction Reactivity of a Scandium(II) Complex, $\{\text{Sc}[\text{N}(\text{SiMe}_3)]\}$. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 2050-2053	16.4	61
89	First-order derivative couplings between excited states from adiabatic TDDFT response theory. <i>Journal of Chemical Physics</i> , 2015 , 142, 064114	3.9	61
88	Analytical First-Order Molecular Properties and Forces within the Adiabatic Connection Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 180-94	6.4	59

87	Accuracy of Electron Affinities of Atoms in Approximate Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 2124-2129	6.4	59
86	(N ₂) ³⁻ radical chemistry via trivalent lanthanide salt/alkali metal reduction of dinitrogen: new syntheses and examples of (N ₂) ²⁻ and (N ₂) ³⁻ complexes and density functional theory comparisons of closed shell Sc ³⁺ , Y ³⁺ , and Lu ³⁺ versus 4f(9) Dy ³⁺ . <i>Inorganic Chemistry</i> , 2011 , 50, 1459-69	5.1	58
85	At What Size Do Neutral Gold Clusters Turn Three-Dimensional?. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 29370-29377	3.8	57
84	Comparisons of lanthanide/actinide +2 ions in a tris(aryloxy)arene coordination environment. <i>Chemical Science</i> , 2017 , 8, 7424-7433	9.4	57
83	Isolation of a radical dianion of nitrogen oxide (NO) ⁽²⁻⁾ . <i>Nature Chemistry</i> , 2010 , 2, 644-7	17.6	57
82	Synthesis, structure, and density functional theory analysis of a scandium dinitrogen complex, [(C(5)Me(4)H)(2)Sc](2)(μ-η(2):η(2)-N(2)). <i>Journal of the American Chemical Society</i> , 2010 , 132, 11151-11158	16.4	54
81	Absolute configuration of D(2)-symmetric fullerene C(84). <i>Journal of the American Chemical Society</i> , 2002 , 124, 3804-5	16.4	54
80	Towards a practical pair density-functional theory for many-electron systems. <i>Physical Review A</i> , 2004 , 70,	2.6	52
79	Mechanism of photocatalytic water oxidation on small TiO nanoparticles. <i>Chemical Science</i> , 2017 , 8, 2179-2183	9.4	50
78	Synthesis, Structure, and Magnetism of Tris(amide) [Ln{N(SiMe) }] Complexes of the Non-traditional +2 Lanthanide Ions. <i>Chemistry - A European Journal</i> , 2018 , 24, 7702-7709	4.8	50
77	Photoelectron spectroscopy of C(84) dianions. <i>Physical Review Letters</i> , 2003 , 91, 113006	7.4	49
76	Structures, C _H and C _H 3 bond energies at borders of polycyclic aromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 5084-5088	3.6	45
75	Insertion of CO ₂ and COS into Bi-C bonds: reactivity of a bismuth NCN pincer complex of an oxyaryl dianionic ligand, [2,6-(Me ₂ NCH ₂) ₂ C ₆ H ₃]Bi(C ₆ H ₂ (t)Bu ₂ O). <i>Journal of the American Chemical Society</i> , 2013 , 135, 7777-87	16.4	44
74	Chapter 2 Time-Dependent Density Functional Theory in Quantum Chemistry. <i>Annual Reports in Computational Chemistry</i> , 2005 , 19-30	1.8	44
73	Isolation of (CO) ¹⁻ and (CO ₂) ¹⁻ radical complexes of rare earths via Ln(NR ₂) ₃ /K reduction and [K ₂ (18-crown-6)] ₂ ⁺ oligomerization. <i>Journal of the American Chemical Society</i> , 2012 , 134, 6064-7	16.4	42
72	Expanding Thorium Hydride Chemistry Through Th ^{III} , Including the Synthesis of a Mixed-Valent Th ^{III} /Th ^{IV} Hydride Complex. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4036-45	16.4	40
71	Direct photolysis of carbonyl compounds dissolved in cloud and fog~droplets. <i>Atmospheric Chemistry and Physics</i> , 2013 , 13, 9461-9477	6.8	40
70	Circular dichroism and conformational dynamics of cepham and their carba and oxa analogues. <i>Chemistry - A European Journal</i> , 2007 , 13, 6732-44	4.8	39

69	Photoelectron spectroscopy of fullerene dianions C ₇₆ (2-), C ₇₈ (2-), and C ₈₄ (2-). <i>Journal of Chemical Physics</i> , 2005 , 122, 094321	3.9	39
68	Ligand Effects in the Synthesis of Ln ²⁺ Complexes by Reduction of Tris(cyclopentadienyl) Precursors Including C≡C Bond Activation of an Indenyl Anion. <i>Organometallics</i> , 2015 , 34, 3909-3921	3.8	36
67	Photodissociation spectroscopy of Ag ₄ (N ₂) _m , m=0-3. <i>Journal of Chemical Physics</i> , 2000 , 113, 5361	3.9	36
66	Light-activated chemical probing of nucleobase solvent accessibility inside cells. <i>Nature Chemical Biology</i> , 2018 , 14, 276-283	11.7	35
65	Tetramethylcyclopentadienyl Ligands Allow Isolation of Ln(II) Ions across the Lanthanide Series in [K(2.2.2-cryptand)][(C ₅ Me ₄ H) ₃ Ln] Complexes. <i>Organometallics</i> , 2018 , 37, 3863-3873	3.8	34
64	Synthesis, Structure, and Reactivity of the Sterically Crowded Th Complex (CMe)Th Including Formation of the Thorium Carbonyl, [(CMe)Th(CO)][BPh]. <i>Journal of the American Chemical Society</i> , 2017 , 139, 3387-3398	16.4	33
63	Accelerating molecular property calculations with nonorthonormal Krylov space methods. <i>Journal of Chemical Physics</i> , 2016 , 144, 174105	3.9	33
62	Metal versus Ligand Reduction in Ln Complexes of a Mesitylene-Anchored Tris(Aryloxo) Ligand. <i>Inorganic Chemistry</i> , 2018 , 57, 2823-2833	5.1	31
61	Faster Energy Transfer and Davydov Splittings in Time-Dependent Density Functional Theory: Lessons from 2-Pyridone Dimer. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 873-80	6.4	30
60	Quadratic Response Properties from TDDFT: Trials and Tribulations. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 807-819	6.4	30
59	Metal effects on ligand non-innocence in Group 5 complexes of the redox-active [ONO] pincer ligand. <i>Dalton Transactions</i> , 2014 , 43, 17991-8000	4.3	29
58	Brominated Luciferins Are Versatile Bioluminescent Probes. <i>ChemBioChem</i> , 2017 , 18, 96-100	3.8	27
57	End-On Bridging Dinitrogen Complex of Scandium. <i>Journal of the American Chemical Society</i> , 2017 , 139, 14861-14864	16.4	27
56	Isolation of +2 rare earth metal ions with three anionic carbocyclic rings: bimetallic bis(cyclopentadienyl) reduced arene complexes of La and Ce are four electron reductants. <i>Chemical Science</i> , 2015 , 6, 7267-7273	9.4	27
55	Synthesis, structure, and physical properties for a series of trigonal bipyramidal M(II)-Cl complexes with intramolecular hydrogen bonds. <i>Dalton Transactions</i> , 2012 , 41, 4358-64	4.3	26
54	Dinitrogen reduction via photochemical activation of heteroleptic tris(cyclopentadienyl) rare-earth complexes. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3804-7	16.4	25
53	Unphysical divergences in response theory. <i>Journal of Chemical Physics</i> , 2016 , 145, 134105	3.9	25
52	Importance of Vibronic Effects in the UV-Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5058-5066	6.4	25

51	Isolation of a Square-Planar Th(III) Complex: Synthesis and Structure of [Th(OCHBu-2,6-Me-4)]. <i>Journal of the American Chemical Society</i> , 2019 , 141, 12458-12463	16.4	23
50	Synthesis of (C5Me5)2(C5Me4H)UMe, (C5Me5)2(C5H5)UMe, and (C5Me5)2UMe[CH(SiMe3)2] from cationic metallocenes for the evaluation of sterically induced reduction. <i>Inorganic Chemistry</i> , 2008 , 47, 10169-76	5.1	23
49	Variational generalized Kohn-Sham approach combining the random-phase-approximation and Green's-function methods. <i>Physical Review A</i> , 2019 , 99,	2.6	22
48	Dinitrogen Reduction, Sulfur Reduction, and Isoprene Polymerization via Photochemical Activation of Trivalent Bis(cyclopentadienyl) Rare-Earth-Metal Allyl Complexes. <i>Organometallics</i> , 2015 , 34, 4387-4393	3.8	21
47	Ring-expanded bicyclic β -lactams: a structure-chiroptical properties relationship investigation by experiment and calculations. <i>Journal of Organic Chemistry</i> , 2011 , 76, 3306-19	4.2	21
46	Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Diels-Alder Chemistry. <i>ACS Chemical Biology</i> , 2019 , 14, 1698-1707	4.9	19
45	Reduction chemistry of the mixed ligand metallocene [(C5Me5)(C8H8)U]2(OC8H8) with bipyridines. <i>Inorganica Chimica Acta</i> , 2010 , 364, 167-171	2.7	19
44	Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18999-19010	3.6	18
43	Asymmetric total synthesis of (+)-fumimycin via 1,2-addition to ketimines. <i>Chemical Communications</i> , 2010 , 46, 9215-7	5.8	18
42	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4185-4190	6.4	18
41	Performance and Scope of Perturbative Corrections to Random-Phase Approximation Energies. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5701-5714	6.4	18
40	Stereochemical Assignment of β -lactam Antibiotics and their Analogues by Electronic Circular Dichroism Spectroscopy. <i>Current Organic Chemistry</i> , 2010 , 14, 1022-1036	1.7	17
39	Divergence of Many-Body Perturbation Theory for Noncovalent Interactions of Large Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2258-2273	6.4	16
38	Solution Synthesis, Structure, and CO2 Reduction Reactivity of a Scandium(II) Complex, {Sc[N(SiMe3)2]3}. <i>Angewandte Chemie</i> , 2017 , 129, 2082-2085	3.6	16
37	Structure of endohedral fullerene Eu@C74. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 6353-8	3.6	16
36	Approximate Density Functionals: Which Should I Choose? 2009 ,		14
35	Au34 in chiral Goldcluster?. <i>Angewandte Chemie</i> , 2007 , 119, 3002-3006	3.6	14
34	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2359-2374	6.4	13

33	Using Diamagnetic Yttrium and Lanthanum Complexes to Explore Ligand Reduction and C-H Bond Activation in a Tris(aryloxy)mesitylene Ligand System. <i>Inorganic Chemistry</i> , 2018 , 57, 12876-12884	5.1	13
32	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5508-5522	6.4	12
31	Trigonal-Planar versus Pyramidal Geometries in the Tris(ring) Heteroleptic Divalent Lanthanide Complexes (C ₅ Me ₅) ₂ Ln(η ³ -Ph) ₂ BPh ₂ : Crystallographic and Density Functional Theory Analysis. <i>Organometallics</i> , 2009 , 28, 6073-6078	3.8	12
30	Differentiating Chemically Similar Lewis Acid Sites in Heterobimetallic Complexes: The Rare-Earth Bridged Hydride (C ₅ Me ₅) ₂ Ln(η ³ -Ph) ₂ Ln'(C ₅ Me ₅) ₂ and Tuckover Hydride (C ₅ Me ₅) ₂ Ln(η ³ -Ph)(η ⁵ -CH ₂ C ₅ Me ₄)Ln'(C ₅ Me ₅) Systems. <i>Organometallics</i> , 2014 , 33, 3882-3890	3.8	11
29	Varying the Lewis base coordination of the Y ₂ N ₂ core in the reduced dinitrogen complexes {(Me ₃ Si) ₂ N} ₂ (LY) ₂ (η ² -N ₂) (L = benzonitrile, pyridines, triphenylphosphine oxide, and trimethylamine N-oxide). <i>Inorganic Chemistry</i> , 2012 , 51, 7867-74	5.1	11
28	Is there symmetry breaking in the first excited singlet state of 2-pyridone dimer?. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 6897-903	2.8	11
27	Chiral cooperativity and solvent-induced tautomerism effects in electronic circular dichroism spectra of [2.2]paracyclophane ketimines. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 6987-93	2.8	11
26	Diastereoselective Coupling of Chiral Acetonide Trisubstituted Radicals with Alkenes. <i>Chemistry - A European Journal</i> , 2016 , 22, 8786-90	4.8	10
25	5-Methoxyquinoline Photobasicity Is Mediated by Water Oxidation. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6645-6651	2.8	10
24	Effective one-particle energies from generalized Kohn-Sham random phase approximation: A direct approach for computing and analyzing core ionization energies. <i>Journal of Chemical Physics</i> , 2019 , 151, 134106	3.9	10
23	Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS-Bridged Dilanthanide Complexes. <i>Journal of the American Chemical Society</i> , 2021 , 143, 8465-8475	16.4	9
22	In search of tris(trimethylsilylcyclopentadienyl) thorium. <i>Dalton Transactions</i> , 2019 , 48, 16633-16640	4.3	9
21	Synthesis of Ln-in-Cryptand Complexes by Chemical Reduction of Ln-in-Cryptand Precursors: Isolation of a Nd-in-Cryptand Complex. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 16141-16146	16.4	9
20	A 9.2-GHz clock transition in a Lu(II) molecular spin qubit arising from a 3,467-MHz hyperfine interaction.. <i>Nature Chemistry</i> , 2022 ,	17.6	9
19	What Is the Price of Open-Source Software?. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2751-4	6.4	8
18	Density functional theory and X-ray analysis of the structural variability in η ³ ,η ³ ,η ³ -tris(ring) rare earth/actinide tetramethylpyrrolyl complexes, (C ₅ Me ₅) ₂ M(NC ₄ Me ₄). <i>Inorganic Chemistry</i> , 2013 , 52, 3565-72	5.1	8
17	Formation of the End-on Bound Lanthanide Dinitrogen Complexes [(RN)Ln-N ₂ -Ln(NR)] from Divalent [(RN)Ln] Salts (R = SiMe). <i>Journal of the American Chemical Society</i> , 2020 , 142, 9302-9313	16.4	6
16	Theoretical Study of Divalent Bis(Pentaisopropylcyclopentadienyl) Actinocenes. <i>Inorganic Chemistry</i> , 2019 , 58, 16004-16010	5.1	6

15	Synthesis and reductive chemistry of bimetallic and trimetallic rare-earth metallocene hydrides with (C ₅ H ₄ SiMe ₃) ₁ ligands. <i>Journal of Organometallic Chemistry</i> , 2017 , 849-850, 38-47	2.3	4
14	C≡C Bond Activation via U(II) in the Reduction of Heteroleptic Bis(trimethylsilyl)amide U(III) Complexes. <i>Organometallics</i> , 2020 , 39, 3425-3432	3.8	4
13	Selfconsistent random phase approximation methods. <i>Journal of Chemical Physics</i> , 2021 , 155, 040902	3.9	4
12	Approximate Density Functionals: Which Should I Choose? 2011 ,		3
11	Theoretische Chemie 2008. <i>Nachrichten Aus Der Chemie</i> , 2009 , 57, 305-311	0.1	3
10	Response Theory and Molecular Properties 2018 , 69-86		3
9	Exploring the Solvation of Acetic Acid in Water Using Liquid Jet X-ray Photoelectron Spectroscopy and Core Level Electron Binding Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 8862-8868	3.4	3
8	Synthesis of a Heteroleptic Pentamethylcyclopentadienyl Yttrium(II) Complex, [K(2.2.2-Cryptand)]{(C ₅ Me ₅) ₂ YII[N(SiMe ₃) ₂]}, and Its C≡C Bond Activated Y(III) Derivative. <i>Organometallics</i> ,	3.8	2
7	Effect of Ammonium Salts on the Decarboxylation of Oxaloacetic Acid in Atmospheric Particles. <i>ACS Earth and Space Chemistry</i> , 2021 , 5, 931-940	3.2	2
6	High-Resolution X-ray Photoelectron Spectroscopy of Organometallic (CHSiMe) ₂ Ln and [(CHSiMe) ₂ Ln] Complexes (Ln = Sm, Eu, Gd, Tb). <i>Journal of the American Chemical Society</i> , 2021 , 143, 16610-16620	16.4	2
5	Synthesis of LnII-in-Cryptand Complexes by Chemical Reduction of LnIII-in-Cryptand Precursors: Isolation of a NdII-in-Cryptand Complex. <i>Angewandte Chemie</i> , 2020 , 132, 16275-16280	3.6	1
4	Density Functional Theory Analysis of the Importance of Coordination Geometry for 5f ₆ d versus 5f ₇ Electron Configurations in U(II) Complexes. <i>Inorganic Chemistry</i> , 2021 , 60, 16316-16325	5.1	1
3	Synthesis of a 2-Isocyanophenolate Ligand, (2-CNC ₆ H ₄ O) ₁ by Ring-Opening of Benzoxazole with Rare-Earth Metal Complexes. <i>Organometallics</i> , 2021 , 40, 735-741	3.8	1
2	Dispersion size-consistency. <i>Electronic Structure</i> , 2022 , 4, 014003	2.6	0
1	Electron correlation methods based on the random phase approximation 2012 , 103-120		