Filipp Furche

List of Publications by Year in Descending Order

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	Dispersion size-consistency. *Electronic Structure*, **2022**, 4, 014003	2.6	0
139	A 9.2-GHz clock transition in a Lu(II) molecular spin qubit arising from a 3,467-MHz hyperfine interaction.. *Nature Chemistry*, **2022**,	17.6	9
138	Density Functional Theory Analysis of the Importance of Coordination Geometry for 5f6d versus 5f Electron Configurations in U(II) Complexes. *Inorganic Chemistry*, **2021**, 60, 16316-16325	5.1	1
137	Effect of Ammonium Salts on the Decarboxylation of Oxaloacetic Acid in Atmospheric Particles. *ACS Earth and Space Chemistry*, **2021**, 5, 931-940	3.2	2
136	Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS-Bridged Dilanthanide Complexes. *Journal of the American Chemical Society*, **2021**, 143, 8465-8475	16.4	9
135	Synthesis of a 2-Isocyanophenolate Ligand, (2-CNC6H4O)1−, by Ring-Opening of Benzoxazole with Rare-Earth Metal Complexes. *Organometallics*, **2021**, 40, 735-741	3.8	1
134	Selfconsistent random phase approximation methods. *Journal of Chemical Physics*, **2021**, 155, 040902	3.9	4
133	Exploring the Solvation of Acetic Acid in Water Using Liquid Jet X-ray Photoelectron Spectroscopy and Core Level Electron Binding Energy Calculations. *Journal of Physical Chemistry B*, **2021**, 125, 8862-8868	3.4	3
132	High-Resolution X-ray Photoelectron Spectroscopy of Organometallic (CHSiMe)Ln and [(CHSiMe)Ln] Complexes (Ln = Sm, Eu, Gd, Tb). *Journal of the American Chemical Society*, **2021**, 143, 16610-16620	16.4	3
131	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107	3.9	255
130	Formation of the End-on Bound Lanthanide Dinitrogen Complexes [(RN)Ln-N?N-Ln(NR)] from Divalent [(RN)Ln] Salts (R = SiMe). *Journal of the American Chemical Society*, **2020**, 142, 9302-9313	16.4	6
129	Synthesis of LnII-in-Cryptand Complexes by Chemical Reduction of LnIII-in-Cryptand Precursors: Isolation of a NdII-in-Cryptand Complex. *Angewandte Chemie*, **2020**, 132, 16275-16280	3.6	1
128	Divergence of Many-Body Perturbation Theory for Noncovalent Interactions of Large Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 2258-2273	6.4	16
127	C−H Bond Activation via U(II) in the Reduction of Heteroleptic Bis(trimethylsilyl)amide U(III) Complexes. *Organometallics*, **2020**, 39, 3425-3432	3.8	4
126	Synthesis of Ln -in-Cryptand Complexes by Chemical Reduction of Ln -in-Cryptand Precursors: Isolation of a Nd -in-Cryptand Complex. *Angewandte Chemie - International Edition*, **2020**, 59, 16141-16146	16.4	9
125	Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation. *Physical Chemistry Chemical Physics*, **2019**, 21, 18999-19010	3.6	18
124	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2019**, 15, 5508-5522	6.4	12

123	Variational generalized Kohn-Sham approach combining the random-phase-approximation and Green's-function methods. *Physical Review A*, **2019**, 99,	2.6	22
122	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. *Journal of Chemical Theory and Computation*, **2019**, 15, 2359-2374	6.4	13
121	Synthesis and Magnetism of Neutral, Linear Metallocene Complexes of Terbium(II) and Dysprosium(II). *Journal of the American Chemical Society*, **2019**, 141, 12967-12973	16.4	109
120	Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Diels-Alder Chemistry. *ACS Chemical Biology*, **2019**, 14, 1698-1707	4.9	19
119	5-Methoxyquinoline Photobasicity Is Mediated by Water Oxidation. *Journal of Physical Chemistry A*, **2019**, 123, 6645-6651	2.8	10
118	Isolation of a Square-Planar Th(III) Complex: Synthesis and Structure of [Th(OCHBu-2,6-Me-4)]. *Journal of the American Chemical Society*, **2019**, 141, 12458-12463	16.4	23
117	Effective one-particle energies from generalized Kohn-Sham random phase approximation: A direct approach for computing and analyzing core ionization energies. *Journal of Chemical Physics*, **2019**, 151, 134106	3.9	10
116	Theoretical Study of Divalent Bis(Pentaisopropylcyclopentadienyl) Actinocenes. *Inorganic Chemistry* , **2019**, 58, 16004-16010	5.1	6
115	In search of tris(trimethylsilylcyclopentadienyl) thorium. *Dalton Transactions*, **2019**, 48, 16633-16640	4.3	9
114	Synthesis, Structure, and Magnetism of Tris(amide) [Ln{N(SiMe) }] Complexes of the Non-traditional +2 Lanthanide Ions. *Chemistry - A European Journal*, **2018**, 24, 7702-7709	4.8	50
113	Metal versus Ligand Reduction in Ln Complexes of a Mesitylene-Anchored Tris(Aryloxide) Ligand. *Inorganic Chemistry*, **2018**, 57, 2823-2833	5.1	31
112	Light-activated chemical probing of nucleobase solvent accessibility inside cells. *Nature Chemical Biology*, **2018**, 14, 276-283	11.7	35
111	Quadratic Response Properties from TDDFT: Trials and Tribulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 807-819	6.4	30
110	Response Theory and Molecular Properties **2018**, 69-86		3
109	Performance and Scope of Perturbative Corrections to Random-Phase Approximation Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 5701-5714	6.4	18
108	Using Diamagnetic Yttrium and Lanthanum Complexes to Explore Ligand Reduction and C-H Bond Activation in a Tris(aryloxide)mesitylene Ligand System. *Inorganic Chemistry*, **2018**, 57, 12876-12884	5.1	13
107	Tetramethylcyclopentadienyl Ligands Allow Isolation of Ln(II) Ions across the Lanthanide Series in [K(2.2.2-cryptand)][(C5Me4H)3Ln] Complexes. *Organometallics*, **2018**, 37, 3863-3873	3.8	34
106	Solution Synthesis, Structure, and CO Reduction Reactivity of a Scandium(II) Complex, {Sc[N(SiMe)] }. *Angewandte Chemie - International Edition*, **2017**, 56, 2050-2053	16.4	61

105	Identification of the Formal +2 Oxidation State of Plutonium: Synthesis and Characterization of {Pu[CH(SiMe)]}. *Journal of the American Chemical Society*, **2017**, 139, 3970-3973	16.4	87
104	Synthesis, Structure, and Reactivity of the Sterically Crowded Th Complex (CMe)Th Including Formation of the Thorium Carbonyl, [(CMe)Th(CO)][BPh]. *Journal of the American Chemical Society*, **2017**, 139, 3387-3398	16.4	33
103	Random-Phase Approximation Methods. *Annual Review of Physical Chemistry*, **2017**, 68, 421-445	15.7	80
102	Brominated Luciferins Are Versatile Bioluminescent Probes. *ChemBioChem*, **2017**, 18, 96-100	3.8	27
101	Mechanism of photocatalytic water oxidation on small TiO nanoparticles. *Chemical Science*, **2017**, 8, 2179-2183	9.4	50
100	End-On Bridging Dinitrogen Complex of Scandium. *Journal of the American Chemical Society*, **2017**, 139, 14861-14864	16.4	27
99	Comparisons of lanthanide/actinide +2 ions in a tris(aryloxide)arene coordination environment. *Chemical Science*, **2017**, 8, 7424-7433	9.4	57
98	Synthesis and reductive chemistry of bimetallic and trimetallic rare-earth metallocene hydrides with (C5H4SiMe3)1□ligands. *Journal of Organometallic Chemistry*, **2017**, 849-850, 38-47	2.3	4
97	Solution Synthesis, Structure, and CO2 Reduction Reactivity of a Scandium(II) Complex, {Sc[N(SiMe3)2]3}□*Angewandte Chemie*, **2017**, 129, 2082-2085	3.6	16
96	Diastereoselective Coupling of Chiral Acetonide Trisubstituted Radicals with Alkenes. *Chemistry - A European Journal*, **2016**, 22, 8786-90	4.8	10
95	Expanding Thorium Hydride Chemistry Through Th□+, Including the Synthesis of a Mixed-Valent Th□/Th□+ Hydride Complex. *Journal of the American Chemical Society*, **2016**, 138, 4036-45	16.4	40
94	Unphysical divergences in response theory. *Journal of Chemical Physics*, **2016**, 145, 134105	3.9	25
93	Accelerating molecular property calculations with nonorthonormal Krylov space methods. *Journal of Chemical Physics*, **2016**, 144, 174105	3.9	33
92	Importance of Vibronic Effects in the UV-Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. *Journal of Chemical Theory and Computation*, **2016**, 12, 5058-5066	6.4	25
91	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. *Journal of Physical Chemistry Letters*, **2016**, 7, 4185-4190	6.4	18
90	First-order derivative couplings between excited states from adiabatic TDDFT response theory. *Journal of Chemical Physics*, **2015**, 142, 064114	3.9	61
89	Ligand Effects in the Synthesis of Ln2+ Complexes by Reduction of Tris(cyclopentadienyl) Precursors Including C□H Bond Activation of an Indenyl Anion. *Organometallics*, **2015**, 34, 3909-3921	3.8	36
88	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8

87	Dinitrogen Reduction, Sulfur Reduction, and Isoprene Polymerization via Photochemical Activation of Trivalent Bis(cyclopentadienyl) Rare-Earth-Metal Allyl Complexes. *Organometallics*, **2015**, 34, 4387-4393	3.8	21
86	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. *Chemical Science*, **2015**, 6, 7267-7273	9.4	27
85	Structural, spectroscopic, and theoretical comparison of traditional vs recently discovered Ln(2+) ions in the [K(2.2.2-cryptand)][(C5H4SiMe3)3Ln] complexes: the variable nature of Dy(2+) and Nd(2+). *Journal of the American Chemical Society*, **2015**, 137, 369-82	16.4	146
84	Synthesis, structure, and reactivity of crystalline molecular complexes of the {[CH(SiMe)]Th} anion containing thorium in the formal +2 oxidation state. *Chemical Science*, **2015**, 6, 517-521	9.4	89
83	Analytical First-Order Molecular Properties and Forces within the Adiabatic Connection Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2014**, 10, 180-94	6.4	59
82	Metal effects on ligand non-innocence in Group 5 complexes of the redox-active [ONO] pincer ligand. *Dalton Transactions*, **2014**, 43, 17991-8000	4.3	29
81	At What Size Do Neutral Gold Clusters Turn Three-Dimensional?. *Journal of Physical Chemistry C*, **2014**, 118, 29370-29377	3.8	57
80	Differentiating Chemically Similar Lewis Acid Sites in Heterobimetallic Complexes: The Rare-Earth Bridged Hydride (C5Me5)2Ln(□H)2Ln?(C5Me5)2 and Tuckover Hydride (C5Me5)2Ln(□H)(□□:□-CH2C5Me4)Ln?(C5Me5) Systems. *Organometallics*, **2014**, 33, 3882-3890	3.8	11
79	Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100	7.9	710
78	Ab initio non-adiabatic molecular dynamics. *Physical Chemistry Chemical Physics*, **2013**, 15, 18336-48	3.6	113
77	Identification of the +2 oxidation state for uranium in a crystalline molecular complex, [K(2.2.2-cryptand)][(C5H4SiMe3)3U]. *Journal of the American Chemical Society*, **2013**, 135, 13310-3	16.4	166
76	Communication: Random phase approximation renormalized many-body perturbation theory. *Journal of Chemical Physics*, **2013**, 139, 171103	3.9	78
75	Dinitrogen reduction via photochemical activation of heteroleptic tris(cyclopentadienyl) rare-earth complexes. *Journal of the American Chemical Society*, **2013**, 135, 3804-7	16.4	25
74	Completing the series of +2 ions for the lanthanide elements: synthesis of molecular complexes of Pr2+, Gd2+, Tb2+, and Lu2+. *Journal of the American Chemical Society*, **2013**, 135, 9857-68	16.4	234
73	Insertion of CO2 and COS into Bi-C bonds: reactivity of a bismuth NCN pincer complex of an oxyaryl dianionic ligand, [2,6-(Me2NCH2)2C6H3]Bi(C6H2(t)Bu2O). *Journal of the American Chemical Society*, **2013**, 135, 7777-87	16.4	44
72	Density functional theory and X-ray analysis of the structural variability in □,□,□-tris(ring) rare earth/actinide tetramethylpyrrolyl complexes, (C5Me5)2M(NC4Me4). *Inorganic Chemistry*, **2013**, 52, 3565-72	5.1	8
71	Direct photolysis of carbonyl compounds dissolved in cloud and fog~droplets. *Atmospheric Chemistry and Physics*, **2013**, 13, 9461-9477	6.8	40
70	Electron correlation methods based on the random phase approximation. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	315

69	Varying the Lewis base coordination of the Y2N2 core in the reduced dinitrogen complexes {[(Me3Si)2N]2(L)Y}2(μ-η2:η2-N2) (L = benzonitrile, pyridines, triphenylphosphine oxide, and trimethylamine N-oxide). *Inorganic Chemistry*, **2012**, 51, 7867-74	5.1	11
68	Expanding rare-earth oxidation state chemistry to molecular complexes of holmium(II) and erbium(II). *Journal of the American Chemical Society*, **2012**, 134, 8420-3	16.4	149
67	Synthesis, structure, and magnetism of an f element nitrosyl complex, (C5Me4H)3UNO. *Journal of the American Chemical Society*, **2012**, 134, 1243-9	16.4	68
66	Synthesis, structure, and physical properties for a series of trigonal bipyramidal M(II)-Cl complexes with intramolecular hydrogen bonds. *Dalton Transactions*, **2012**, 41, 4358-64	4.3	26
65	Isolation of (CO)1- and (CO2)1- radical complexes of rare earths via Ln(NR2)3/K reduction and [K2(18-crown-6)2]2+ oligomerization. *Journal of the American Chemical Society*, **2012**, 134, 6064-7	16.4	42
64	Circular dichroism: electronic. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 150-166	7.9	81
63	Harnessing the meta-generalized gradient approximation for time-dependent density functional theory. *Journal of Chemical Physics*, **2012**, 137, 164105	3.9	75
62	Basis set convergence of molecular correlation energy differences within the random phase approximation. *Journal of Chemical Physics*, **2012**, 136, 084105	3.9	81
61	Electron correlation methods based on the random phase approximation **2012**, 103-120		
60	Approximate Density Functionals: Which Should I Choose? **2011**,		3
59	A Parameter-Free Density Functional That Works for Noncovalent Interactions. *Journal of Physical Chemistry Letters*, **2011**, 2, 983-989	6.4	124
58	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 20986-98	3.6	71
57	Facile bismuth-oxygen bond cleavage, C-H activation, and formation of a monodentate carbon-bound oxyaryl dianion, (CH(t)Bu)3Bi,5-O-4)2. *Journal of the American Chemical Society*, **2011**, 133, 5244-7	16.4	74
56	Ring-expanded bicyclic β-lactams: a structure-chiroptical properties relationship investigation by experiment and calculations. *Journal of Organic Chemistry*, **2011**, 76, 3306-19	4.2	21
55	Assessing Excited State Methods by Adiabatic Excitation Energies. *Journal of Chemical Theory and Computation*, **2011**, 7, 2376-86	6.4	146
54	Synthesis of the (N2)3- radical from Y2+ and its protonolysis reactivity to form (N2H2)2- via the Y[N(SiMe3)2]3/KC8 reduction system. *Journal of the American Chemical Society*, **2011**, 133, 3784-7	16.4	63
53	(N2)3- radical chemistry via trivalent lanthanide salt/alkali metal reduction of dinitrogen: new syntheses and examples of (N2)2- and (N2)3- complexes and density functional theory comparisons of closed shell Sc3+, Y3+, and Lu3+ versus 4f(9) Dy3+. *Inorganic Chemistry*, **2011**, 50, 1459-69	5.1	58
52	Isolation of a radical dianion of nitrogen oxide (NO)(2-). *Nature Chemistry*, **2010**, 2, 644-7	17.6	57

51	Accuracy of Electron Affinities of Atoms in Approximate Density Functional Theory. *Journal of Physical Chemistry Letters*, **2010**, 1, 2124-2129	6.4	59
50	Synthesis, structure, and density functional theory analysis of a scandium dinitrogen complex, [(C(5)Me(4)H)(2)Sc](2)(mu-eta(2):eta(2)-N(2)). *Journal of the American Chemical Society*, **2010**, 132, 11151-8	16.4	54
49	Is there symmetry breaking in the first excited singlet state of 2-pyridone dimer?. *Journal of Physical Chemistry A*, **2010**, 114, 6897-903	2.8	11
48	First-order nonadiabatic couplings from time-dependent hybrid density functional response theory: Consistent formalism, implementation, and performance. *Journal of Chemical Physics*, **2010**, 132, 044107	3.9	174
47	Asymmetric total synthesis of (+)-fumimycin via 1,2-addition to ketimines. *Chemical Communications*, **2010**, 46, 9215-7	5.8	18
46	Fast computation of molecular random phase approximation correlation energies using resolution of the identity and imaginary frequency integration. *Journal of Chemical Physics*, **2010**, 132, 234114	3.9	190
45	Stereochemical Assingment of β -lactam Antibiotics and their Analogues by Electronic Circular Dichroism Spectroscopy. *Current Organic Chemistry*, **2010**, 14, 1022-1036	1.7	17
44	Property-optimized gaussian basis sets for molecular response calculations. *Journal of Chemical Physics*, **2010**, 133, 134105	3.9	1040
43	Reduction chemistry of the mixed ligand metallocene [(C5Me5)(C8H8)U]2(□C8H8) with bipyridines. *Inorganica Chimica Acta*, **2010**, 364, 167-171	2.7	19
42	Approximate Density Functionals: Which Should I Choose? **2009**,		14
41	F□ster Energy Transfer and Davydov Splittings in Time-Dependent Density Functional Theory: Lessons from 2-Pyridone Dimer. *Journal of Chemical Theory and Computation*, **2009**, 5, 873-80	6.4	30
40	Trigonal-Planar versus Pyramidal Geometries in the Tris(ring) Heteroleptic Divalent Lanthanide Complexes (C5Me5)Ln(□6:□1-Ph)2BPh2: Crystallographic and Density Functional Theory Analysis. *Organometallics*, **2009**, 28, 6073-6078	3.8	12
39	Theoretische Chemie 2008. *Nachrichten Aus Der Chemie*, **2009**, 57, 305-311	0.1	3
38	Chiral cooperativity and solvent-induced tautomerism effects in electronic circular dichroism spectra of [2.2]paracyclophane ketimines. *Journal of Physical Chemistry A*, **2009**, 113, 6987-93	2.8	11
37	Excited States from Time-Dependent Density Functional Theory. *Reviews in Computational Chemistry*, **2009**, 91-165		115
36	Structure of endohedral fullerene Eu@C74. *Physical Chemistry Chemical Physics*, **2009**, 11, 6353-8	3.6	16
35	Isolation of dysprosium and yttrium complexes of a three-electron reduction product in the activation of dinitrogen, the (N2)3- radical. *Journal of the American Chemical Society*, **2009**, 131, 11195-202	16.4	99
34	2D-3D transition of gold cluster anions resolved. *Physical Review A*, **2008**, 77,	2.6	243

33	Developing the random phase approximation into a practical post-Kohn-Sham correlation model. *Journal of Chemical Physics*, **2008**, 129, 114105	3.9	223
32	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. *Inorganic Chemistry*, **2008**, 47, 10169-76	5.1	23
31	Au34-: a chiral gold cluster?. *Angewandte Chemie - International Edition*, **2007**, 46, 2944-8	16.4	127
30	Au34□ein chiraler Goldcluster?. *Angewandte Chemie*, **2007**, 119, 3002-3006	3.6	14
29	Lagrangian approach to molecular vibrational Raman intensities using time-dependent hybrid density functional theory. *Journal of Chemical Physics*, **2007**, 126, 201104	3.9	71
28	Circular dichroism and conformational dynamics of cephams and their carba and oxa analogues. *Chemistry - A European Journal*, **2007**, 13, 6732-44	4.8	39
27	The performance of semilocal and hybrid density functionals in 3d transition-metal chemistry. *Journal of Chemical Physics*, **2006**, 124, 044103	3.9	488
26	Analytical time-dependent density functional derivative methods within the RI-J approximation, an approach to excited states of large molecules. *Journal of Chemical Physics*, **2005**, 122, 064105	3.9	119
25	Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. *Theoretical and Computational Chemistry*, **2005**, 16, 93-128		169
24	Fluctuation-dissipation theorem density-functional theory. *Journal of Chemical Physics*, **2005**, 122, 164106	3.9	180
23	Photoelectron spectroscopy of fullerene dianions C76(2-), C78(2-), and C84(2-). *Journal of Chemical Physics*, **2005**, 122, 094321	3.9	39
22	Chapter 2 Time-Dependent Density Functional Theoryin Quantum Chemistry. *Annual Reports in Computational Chemistry*, **2005**, 19-30	1.8	44
21	Nuclear second analytical derivative calculations using auxiliary basis set expansions. *Chemical Physics Letters*, **2004**, 384, 103-107	2.5	326
20	Electronic photodissociation spectroscopy of Aun- x Xe (n = 7-11) versus time-dependent density functional theory prediction. *Journal of Chemical Physics*, **2004**, 121, 4619-27	3.9	66
19	Photoinduced intramolecular charge transfer in 4-(dimethyl)aminobenzonitrile--a theoretical perspective. *Journal of the American Chemical Society*, **2004**, 126, 1277-84	16.4	230
18	Towards a practical pair density-functional theory for many-electron systems. *Physical Review A*, **2004**, 70,	2.6	52
17	Gaussian basis sets of quadruple zeta valence quality for atoms HKr. *Journal of Chemical Physics*, **2003**, 119, 12753-12762	3.9	784
16	Photoelectron spectroscopy of C(84) dianions. *Physical Review Letters*, **2003**, 91, 113006	7.4	49

15	An improved method for density functional calculations of the frequency-dependent optical rotation. *Chemical Physics Letters*, **2002**, 361, 321-328	2.5	175
14	An efficient implementation of second analytical derivatives for density functional methods. *Chemical Physics Letters*, **2002**, 362, 511-518	2.5	520
13	Adiabatic time-dependent density functional methods for excited state properties. *Journal of Chemical Physics*, **2002**, 117, 7433-7447	3.9	1777
12	Structures of small gold cluster cations (Aun+, n. *Journal of Chemical Physics*, **2002**, 116, 4094-4101	3.9	422
11	Efficient characterization of stationary points on potential energy surfaces. *Journal of Chemical Physics*, **2002**, 117, 9535-9538	3.9	233
10	The structures of small gold cluster anions as determined by a combination of ion mobility measurements and density functional calculations. *Journal of Chemical Physics*, **2002**, 117, 6982-6990	3.9	498
9	Absolute configuration of D(2)-symmetric fullerene C(84). *Journal of the American Chemical Society*, **2002**, 124, 3804-5	16.4	54
8	Molecular tests of the random phase approximation to the exchange-correlation energy functional. *Physical Review B*, **2001**, 64,	3.3	360
7	On the density matrix based approach to time-dependent density functional response theory. *Journal of Chemical Physics*, **2001**, 114, 5982-5992	3.9	349
6	Fullerene C80: Are there still more isomers?. *Journal of Chemical Physics*, **2001**, 114, 10362-10367	3.9	63
5	Comment on Assessment of exchange correlation functionals[A.J. Cohen, N.C. Handy, Chem. Phys. Lett. 316 (2000) 160166]. *Chemical Physics Letters*, **2000**, 325, 317-321	2.5	70
4	Structures, CH and CCH3 bond energies at borders of polycyclic aromatic hydrocarbons. *Physical Chemistry Chemical Physics*, **2000**, 2, 5084-5088	3.6	45
3	Photodissociation spectroscopy of Ag4+(N2)m, m=04. *Journal of Chemical Physics*, **2000**, 113, 5361	3.9	36
2	Circular Dichroism of Helicenes Investigated by Time-Dependent Density Functional Theory. *Journal of the American Chemical Society*, **2000**, 122, 1717-1724	16.4	431
1	Synthesis of a Heteroleptic Pentamethylcyclopentadienyl Yttrium(II) Complex, [K(2.2.2-Cryptand)]{(C5Me5)2YII[N(SiMe3)2]}, and Its CH Bond Activated Y(III) Derivative. *Organometallics*,	3.8	2