Filipp Furche

List of Publications by Year
in descending order

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140 papers	18,307 citations	20759 60 h-index	12233 133 g-index
155 all docs	155 docs citations	155 times ranked	12786 citing authors

#	Article	IF	Citations
1	2.2.2-Cryptand complexes of neptunium(<scp>iii</scp>) and plutonium(<scp>iii</scp>). Chemical Communications, 2022, 58, 997-1000.	2.2	8
2	Dispersion size-consistency. Electronic Structure, 2022, 4, 014003.	1.0	3
3	A 9.2-GHz clock transition in a Lu(II) molecular spin qubit arising from a 3,467-MHz hyperfine interaction. Nature Chemistry, 2022, 14, 392-397.	6.6	43
4	Synthesis and Reduction of Heteroleptic Bis(cyclopentadienyl) Uranium(III) Complexes. Inorganic Chemistry, 2022, 61, 7365-7376.	1.9	16
5	Synthesis of a 2-Isocyanophenolate Ligand, (2-CNC₆H₄O)^{1â€“}, by Ring-Opening of Benzoxazole with Rare-Earth Metal Complexes. Organometallics, 2021, 40, 735-741.	1.1	3
6	Effect of Ammonium Salts on the Decarboxylation of Oxaloacetic Acid in Atmospheric Particles. ACS Earth and Space Chemistry, 2021, 5, 931-940.	1.2	2
7	Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS₄³^{â€“}-Bridged Dilanthanide Complexes. Journal of the American Chemical Society, 2021, 143, 8465-8475.	6.6	27
8	Selfconsistent random phase approximation methods. Journal of Chemical Physics, 2021, 155, 040902.	1.2	16
9	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.	1.2	6
10	High-Resolution X-ray Photoelectron Spectroscopy of Organometallic (C₅H₄SiMe₃)₃Ln^{III} and [(C₅H₄SiMe₃)₃Ln^{II}]^{1â€“} Complexes (Ln = Sm, Eu, Gd, Tb). Journal of the American Chemical Society, 2021, 143, 16610-16620.	6.6	17
11	Density Functional Theory Analysis of the Importance of Coordination Geometry for 5f³6d¹ versus 5f⁴ Electron Configurations in U(II) Complexes. Inorganic Chemistry, 2021, 60, 16316-16325.	1.9	6
12	Synthesis of a Heteroleptic Pentamethylcyclopentadienyl Yttrium(II) Complex, [K(2.2.2-Cryptand)]{(C₅Me₅)₂Y^{II}[N(SiMe₃)₂]}, and Its Câ€“H Bond Activated Y(III) Derivative. Organometallics, 2021, 40, 3917-3925.	1.1	8
13	Câ€“H Bond Activation via U(II) in the Reduction of Heteroleptic Bis(trimethylsilyl)amide U(III) Complexes. Organometallics, 2020, 39, 3425-3432.	1.1	17
14	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
15	Formation of the End-on Bound Lanthanide Dinitrogen Complexes [(R₂N)₃Lnâ€“Nâ€“Nâ€“Ln(NR₂)₃]^{2â€“} from Divalent [(R₂N)₃Ln]^{1â€“} Salts (R = SiMe₃). Journal of the American Chemical Society, 2020, 142, 9302-9313.	6.6	15
16	Synthesis of Ln II â€inâ€Cryptand Complexes by Chemical Reduction of Ln III â€inâ€Cryptand Precursors: Isolation of a Nd II â€inâ€Cryptand Complex. Angewandte Chemie, 2020, 132, 16275-16280.	1.6	3
17	Divergence of Many-Body Perturbation Theory for Noncovalent Interactions of Large Molecules. Journal of Chemical Theory and Computation, 2020, 16, 2258-2273.	2.3	39
18	Synthesis of Ln^{II}â€inâ€Cryptand Complexes by Chemical Reduction of Ln^{III}â€inâ€Cryptand Precursors: Isolation of a Nd^{II}â€inâ€Cryptand Complex. Angewandte Chemie - International Edition, 2020, 59, 16141-16146.	7.2	18

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19	Synthesis and Magnetism of Neutral, Linear Metallocene Complexes of Terbium(II) and Dysprosium(II). Journal of the American Chemical Society, 2019, 141, 12967-12973.	6.6	186
20	Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Dielsâ€“Alder Chemistry. ACS Chemical Biology, 2019, 14, 1698-1707.	1.6	36
21	5-Methoxyquinoline Photobasicity Is Mediated by Water Oxidation. Journal of Physical Chemistry A, 2019, 123, 6645-6651.	1.1	15
22	Isolation of a Square-Planar Th(III) Complex: Synthesis and Structure of [Th(OC₆H₂^tBu₂-2,6-Me-4)₄]^{1â€“}. Journal of the American Chemical Society, 2019, 141, 12458-12463.	6.6	42
23	Effective one-particle energies from generalized Kohnâ€“Sham random phase approximation: A direct approach for computing and analyzing core ionization energies. Journal of Chemical Physics, 2019, 151, 134106.	1.2	16
24	Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation. Physical Chemistry Chemical Physics, 2019, 21, 18999-19010.	1.3	31
25	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2019, 15, 5508-5522.	2.3	21
26	Variational generalized Kohn-Sham approach combining the random-phase-approximation and Green's-function methods. Physical Review A, 2019, 99, .	1.0	39
27	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.	2.3	18
28	Theoretical Study of Divalent Bis(Pentaisopropylcyclopentadienyl) Actinocenes. Inorganic Chemistry, 2019, 58, 16004-16010.	1.9	10
29	In search of tris(trimethylsilylcyclopentadienyl) thorium. Dalton Transactions, 2019, 48, 16633-16640.	1.6	18
30	Synthesis, Structure, and Magnetism of Tris(amide) [Ln{N(SiMe₃)₂}₃]^{1â^’} Complexes of the Nonâ€traditional +2 Lanthanide Ions. Chemistry - A European Journal, 2018, 24, 7702-7709.	1.7	64
31	Metal versus Ligand Reduction in Ln³⁺ Complexes of a Mesitylene-Anchored Tris(Aryloxide) Ligand. Inorganic Chemistry, 2018, 57, 2823-2833.	1.9	41
32	Light-activated chemical probing of nucleobase solvent accessibility inside cells. Nature Chemical Biology, 2018, 14, 276-283.	3.9	47
33	Quadratic Response Properties from TDDFT: Trials and Tribulations. Journal of Chemical Theory and Computation, 2018, 14, 807-819.	2.3	49
34	Response Theory and Molecular Properties. , 2018, , 69-86.		5
35	Performance and Scope of Perturbative Corrections to Random-Phase Approximation Energies. Journal of Chemical Theory and Computation, 2018, 14, 5701-5714.	2.3	23
36	Using Diamagnetic Yttrium and Lanthanum Complexes to Explore Ligand Reduction and Câ€“H Bond Activation in a Tris(aryloxide)mesitylene Ligand System. Inorganic Chemistry, 2018, 57, 12876-12884.	1.9	15

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37	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.	1.1	46
38	Solution Synthesis, Structure, and CO₂ Reduction Reactivity of a Scandium(II) Complex, {Sc[N(SiMe₃)₂]₃}^{â^'}. Angewandte Chemie - International Edition, 2017, 56, 2050-2053.	7.2	75
39	Identification of the Formal +2 Oxidation State of Plutonium: Synthesis and Characterization of {Pu^{II}[C₅H₃(SiMe₃)₂]₃}^{â^'}. Journal of the American Chemical Society, 2017, 139, 3970-3973.	6.6	121
40	Synthesis, Structure, and Reactivity of the Sterically Crowded Th³⁺ Complex (C₅Me₅)₃Th Including Formation of the Thorium Carbonyl, [(C₅Me₅)₃Th(CO)][BPh₄]. Journal of the American Chemical Society, 2017, 139, 3387-3398.	6.6	51
41	Random-Phase Approximation Methods. Annual Review of Physical Chemistry, 2017, 68, 421-445.	4.8	127
42	Brominated Luciferins Are Versatile Bioluminescent Probes. ChemBioChem, 2017, 18, 96-100.	1.3	35
43	Mechanism of photocatalytic water oxidation on small TiO₂ nanoparticles. Chemical Science, 2017, 8, 2179-2183.	3.7	59
44	End-On Bridging Dinitrogen Complex of Scandium. Journal of the American Chemical Society, 2017, 139, 14861-14864.	6.6	38
45	Comparisons of lanthanide/actinide +2 ions in a tris(aryloxide)arene coordination environment. Chemical Science, 2017, 8, 7424-7433.	3.7	70
46	Synthesis and reductive chemistry of bimetallic and trimetallic rare-earth metallocene hydrides with (C5H4SiMe3)1â^' ligands. Journal of Organometallic Chemistry, 2017, 849-850, 38-47.	0.8	8
47	Solution Synthesis, Structure, and CO₂ Reduction Reactivity of a Scandium(II) Complex, {Sc[N(SiMe₃)₂]₃}^{â^'}. Angewandte Chemie, 2017, 129, 2082-2085.	1.6	21
48	Unphysical divergences in response theory. Journal of Chemical Physics, 2016, 145, 134105.	1.2	35
49	Accelerating molecular property calculations with nonorthonormal Krylov space methods. Journal of Chemical Physics, 2016, 144, 174105.	1.2	50
50	Importance of Vibronic Effects in the UVâ€“Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. Journal of Chemical Theory and Computation, 2016, 12, 5058-5066.	2.3	35
51	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. Journal of Physical Chemistry Letters, 2016, 7, 4185-4190.	2.1	21
52	Diastereoselective Coupling of Chiral Acetonide Trisubstituted Radicals with Alkenes. Chemistry - A European Journal, 2016, 22, 8786-8790.	1.7	12
53	Expanding Thorium Hydride Chemistry Through Th²⁺, Including the Synthesis of a Mixed-Valent Th⁴⁺/Th³⁺ Hydride Complex. Journal of the American Chemical Society, 2016, 138, 4036-4045.	6.6	59
54	Isolation of +2 rare earth metal ions with three anionic carbocyclic rings: bimetallic bis(cyclopentadienyl) reduced arene complexes of La²⁺ and Ce²⁺ are four electron reductants. Chemical Science, 2015, 6, 7267-7273.	3.7	38

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55	Structural, Spectroscopic, and Theoretical Comparison of Traditional vs Recently Discovered Ln²⁺ Ions in the [K(2.2.2-cryptand)][(C₅H₄SiMe₃)₃Ln] Complexes: The Variable Nature of Dy²⁺ and Nd²⁺. Journal of the American Chemical Society, 2015, 137, 369-382.	6.6	185
56	Synthesis, structure, and reactivity of crystalline molecular complexes of the {[C₅H₃(SiMe₃)₂]₃Th}^{1â^'} anion containing thorium in the formal +2 oxidation state. Chemical Science, 2015, 6, 517-521.	3.7	119
57	First-order derivative couplings between excited states from adiabatic TDDFT response theory. Journal of Chemical Physics, 2015, 142, 064114.	1.2	86
58	Ligand Effects in the Synthesis of Ln²⁺ Complexes by Reduction of Tris(cyclopentadienyl) Precursors Including Câ€“H Bond Activation of an Indenyl Anion. Organometallics, 2015, 34, 3909-3921.	1.1	40
59	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	2.1	19
60	Dinitrogen Reduction, Sulfur Reduction, and Isoprene Polymerization via Photochemical Activation of Trivalent Bis(cyclopentadienyl) Rare-Earth-Metal Allyl Complexes. Organometallics, 2015, 34, 4387-4393.	1.1	28
61	Turbomole. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 91-100.	6.2	867
62	Analytical First-Order Molecular Properties and Forces within the Adiabatic Connection Random Phase Approximation. Journal of Chemical Theory and Computation, 2014, 10, 180-194.	2.3	73
63	Metal effects on ligand non-innocence in Group 5 complexes of the redox-active [ONO] pincer ligand. Dalton Transactions, 2014, 43, 17991-18000.	1.6	32
64	At What Size Do Neutral Gold Clusters Turn Three-Dimensional?. Journal of Physical Chemistry C, 2014, 118, 29370-29377.	1.5	70
65	Differentiating Chemically Similar Lewis Acid Sites in Heterobimetallic Complexes: The Rare-Earth Bridged Hydride (C₅Me₅)₂Ln(Î¼-H)₂Lnâ€²(C₅Me₅)₂ and Tuckover Hydride (C₅Me₅)₂Ln(Î¼-H)(Î¼-Î·¹:Î·⁵-CH₂C₅Me₄) Systems. Organometallics, 2014, 33, 3882-3890.	1.1	14
66	Ab initio non-adiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 18336.	1.3	145
67	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, 13310-13313.	6.6	220
68	Communication: Random phase approximation renormalized many-body perturbation theory. Journal of Chemical Physics, 2013, 139, 171103.	1.2	93
69	Dinitrogen Reduction via Photochemical Activation of Heteroleptic Tris(cyclopentadienyl) Rare-Earth Complexes. Journal of the American Chemical Society, 2013, 135, 3804-3807.	6.6	31
70	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, 9857-9868.	6.6	292
71	Insertion of CO₂ and COS into Biâ€“C Bonds: Reactivity of a Bismuth NCN Pincer Complex of an Oxyaryl Dianionic Ligand, [2,6-(Me₂NCH₂)₂C₆H₃]Bi(C₆H₂<sup><i	6.6	56
72	Journal of the American Chemical Society, 2013, 135, 7777-7787. Density Functional Theory and X-ray Analysis of the Structural Variability in Î·⁵,Î·⁵,Î·¹-Tris(ring) Rare Earth/Actinide Tetramethylpyrrolyl Complexes, (C₅Me₅)₂M(NC₄Me₄). Inorganic Chemistry, 2013, 52, 3565-3572.	1.9	11

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73	Direct photolysis of carbonyl compounds dissolved in cloud and fog~droplets. Atmospheric Chemistry and Physics, 2013, 13, 9461-9477.	1.9	44
74	Harnessing the meta-generalized gradient approximation for time-dependent density functional theory. Journal of Chemical Physics, 2012, 137, 164105.	1.2	101
75	Basis set convergence of molecular correlation energy differences within the random phase approximation. Journal of Chemical Physics, 2012, 136, 084105.	1.2	92
76	Varying the Lewis Base Coordination of the Y₂N₂ Core in the Reduced Dinitrogen Complexes {[(Me₃Si)₂N]₂(L)Y}₂(Î¼-Î·²:Î·²-N₂) (L = Benzonitrile, Pyridines, Triphenylphosphine Oxide, and Trimethylamine N-Oxide). Inorganic Chemistry, 2012, 51, 7867-7874.	1.9	18
77	Expanding Rare-Earth Oxidation State Chemistry to Molecular Complexes of Holmium(II) and Erbium(II). Journal of the American Chemical Society, 2012, 134, 8420-8423.	6.6	182
78	Synthesis, Structure, and Magnetism of an f Element Nitrosyl Complex, (C5Me4H)3UNO. Journal of the American Chemical Society, 2012, 134, 1243-1249.	6.6	69
79	Computational Modeling of Excitation Energy Transfer in Xanthorhodopsin, a Model Light-Harvesting System. Biophysical Journal, 2012, 102, 167a.	0.2	0
80	Synthesis, structure, and physical properties for a series of trigonal bipyramidal MIIâ€“Cl complexes with intramolecular hydrogen bonds. Dalton Transactions, 2012, 41, 4358.	1.6	27
81	Isolation of (CO)^{1â€“} and (CO₂)^{1â€“} 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, 6064-6067.	6.6	53
82	Circular dichroism: electronic. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 150-166.	6.2	106
83	Electron correlation methods based on the random phase approximation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	353
84	Electron correlation methods based on the random phase approximation. , 2012, , 103-120.		0
85	(N₂)^{3â€“} Radical Chemistry via Trivalent Lanthanide Salt/Alkali Metal Reduction of Dinitrogen: New Syntheses and Examples of (N₂)^{2â€“} and (N₂)^{3â€“} Complexes and Density Functional Theory Comparisons of Closed Shell Sc³⁺, Y³⁺, and Lu³⁺ versus 4f⁹ Dy³⁺. Inorganic Chemistry, 2011, 50, 1459-1469.	1.9	65
86	A Parameter-Free Density Functional That Works for Noncovalent Interactions. Journal of Physical Chemistry Letters, 2011, 2, 983-989.	2.1	134
87	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 20986.	1.3	87
88	Facile Bismuthâ€“Oxygen Bond Cleavage, Câ€“H Activation, and Formation of a Monodentate Carbon-Bound Oxyaryl Dianion, (C₆H₂^tBu₂-3,5-O-4)^{2â€“}. Journal of the American Chemical Society, 2011, 133, 5244-5247.	6.6	86
89	Ring-Expanded Bicyclic Î²-Lactams: A Structureâ€“Chiroptical Properties Relationship Investigation by Experiment and Calculations. Journal of Organic Chemistry, 2011, 76, 3306-3319.	1.7	23
90	Assessing Excited State Methods by Adiabatic Excitation Energies. Journal of Chemical Theory and Computation, 2011, 7, 2376-2386.	2.3	164

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91	Synthesis of the (N₂)^{3â^'} Radical from Y²⁺ and Its Protonolysis Reactivity To Form (N₂H₂)^{2â^'} via the Y[N(SiMe₃)₂]₃/KC₈ Reduction System. Journal of the American Chemical Society, 2011, 133, 3784-3787.	6.6	75
92	Stereochemical Assingment of β -lactam Antibiotics and their Analogues by Electronic Circular Dichroism Spectroscopy. Current Organic Chemistry, 2010, 14, 1022-1036.	0.9	19
93	Property-optimized Gaussian basis sets for molecular response calculations. Journal of Chemical Physics, 2010, 133, 134105.	1.2	1,357
94	Reduction chemistry of the mixed ligand metallocene [(C5Me5)(C8H8)U]2(Î¼-C8H8) with bipyridines. Inorganica Chimica Acta, 2010, 364, 167-171.	1.2	22
95	Isolation of a radical dianion of nitrogen oxide (NO)2â^'. Nature Chemistry, 2010, 2, 644-647.	6.6	64
96	Tackling Non-Adiabatic Effects by Time-Dependent Density Functional Theory. , 2010, , .		0
97	Accuracy of Electron Affinities of Atoms in Approximate Density Functional Theory. Journal of Physical Chemistry Letters, 2010, 1, 2124-2129.	2.1	66
98	Synthesis, Structure, and Density Functional Theory Analysis of a Scandium Dinitrogen Complex, [(C₅Me₄H)₂Sc]₂(Î¼-Î·²:Î·²-N₂). Journal of the American Chemical Society, 2010, 132, 11151-11158.	6.6	62
99	Is There Symmetry Breaking in the First Excited Singlet State of 2-Pyridone Dimer?. Journal of Physical Chemistry A, 2010, 114, 6897-6903.	1.1	11
100	First-order nonadiabatic couplings from time-dependent hybrid density functional response theory: Consistent formalism, implementation, and performance. Journal of Chemical Physics, 2010, 132, 044107.	1.2	207
101	Asymmetric total synthesis of (+)-fumimycin via 1,2-addition to ketimines. Chemical Communications, 2010, 46, 9215.	2.2	22
102	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.	1.2	228
103	FÃ¶rster Energy Transfer and Davydov Splittings in Time-Dependent Density Functional Theory: Lessons from 2-Pyridone Dimer. Journal of Chemical Theory and Computation, 2009, 5, 873-880.	2.3	32
104	Trigonal-Planar versus Pyramidal Geometries in the Tris(ring) Heteroleptic Divalent Lanthanide Complexes (C₅Me₅)Ln(Î¼-Î·⁶:Î·¹-Ph)₂BPh₂: Crystallographic and Density Functional Theory Analysis. Organometallics, 2009, 28, 6073-6078.	1.1	14
105	Theoretische Chemie 2008. Nachrichten Aus Der Chemie, 2009, 57, 305-311.	0.0	4
106	Chiral Cooperativity and Solvent-Induced Tautomerism Effects in Electronic Circular Dichroism Spectra of [2.2]Paracyclophane Ketimines. Journal of Physical Chemistry A, 2009, 113, 6987-6993.	1.1	11
107	Structure of endohedral fullerene Eu@C74. Physical Chemistry Chemical Physics, 2009, 11, 6353.	1.3	17
108	Isolation of Dysprosium and Yttrium Complexes of a Three-Electron Reduction Product in the Activation of Dinitrogen, the (N₂)^{3â^'} Radical. Journal of the American Chemical Society, 2009, 131, 11195-11202.	6.6	117

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109	2D-3D transition of gold cluster anions resolved. Physical Review A, 2008, 77, .	1.0	255
110	Developing the random phase approximation into a practical post-Kohnâ€“Sham correlation model. Journal of Chemical Physics, 2008, 129, 114105.	1.2	246
111	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, 10169-10176.	1.9	26
112	Lagrangian approach to molecular vibrational Raman intensities using time-dependent hybrid density functional theory. Journal of Chemical Physics, 2007, 126, 201104.	1.2	77
113	Circular Dichroism and Conformational Dynamics of Cephams and Their Carba and Oxa Analogues. Chemistry - A European Journal, 2007, 13, 6732-6744.	1.7	41
114	Au34â^': A Chiral Gold Cluster?. Angewandte Chemie - International Edition, 2007, 46, 2944-2948.	7.2	139
115	The performance of semilocal and hybrid density functionals in 3d transition-metal chemistry. Journal of Chemical Physics, 2006, 124, 044103.	1.2	528
116	Photoelectron spectroscopy of fullerene dianions C762â^', C782â^', and C842â^'. Journal of Chemical Physics, 2005, 122, 094321.	1.2	39
117	Chapter 2 Time-Dependent Density Functional Theoryin Quantum Chemistry. Annual Reports in Computational Chemistry, 2005, , 19-30.	0.9	48
118	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.	1.2	130
119	Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. Theoretical and Computational Chemistry, 2005, 16, 93-128.	0.2	192
120	Fluctuation-dissipation theorem density-functional theory. Journal of Chemical Physics, 2005, 122, 164106.	1.2	196
121	Nuclear second analytical derivative calculations using auxiliary basis set expansions. Chemical Physics Letters, 2004, 384, 103-107.	1.2	364
122	Electronic photodissociation spectroscopy of Aunâ^'â‹…Xeâ€Š(n=7â€“11) versus time-dependent density functional theory prediction. Journal of Chemical Physics, 2004, 121, 4619-4627.	1.2	72
123	Photoinduced Intramolecular Charge Transfer in 4-(Dimethyl)aminobenzonitrile â^' A Theoretical Perspective. Journal of the American Chemical Society, 2004, 126, 1277-1284.	6.6	244
124	Towards a practical pair density-functional theory for many-electron systems. Physical Review A, 2004, 70, .	1.0	58
125	Gaussian basis sets of quadruple zeta valence quality for atoms Hâ€“Kr. Journal of Chemical Physics, 2003, 119, 12753-12762.	1.2	946
126	Photoelectron Spectroscopy ofC84Dianions. Physical Review Letters, 2003, 91, 113006.	2.9	50

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127	Structures of small gold cluster cations (Aun+, n<14): Ion mobility measurements versus density functional calculations. Journal of Chemical Physics, 2002, 116, 4094-4101.	1.2	441
128	Efficient characterization of stationary points on potential energy surfaces. Journal of Chemical Physics, 2002, 117, 9535-9538.	1.2	253
129	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.	1.2	524
130	Absolute Configuration ofD2-Symmetric Fullerene C84. Journal of the American Chemical Society, 2002, 124, 3804-3805.	6.6	55
131	An improved method for density functional calculations of the frequency-dependent optical rotation. Chemical Physics Letters, 2002, 361, 321-328.	1.2	189
132	An efficient implementation of second analytical derivatives for density functional methods. Chemical Physics Letters, 2002, 362, 511-518.	1.2	561
133	Adiabatic time-dependent density functional methods for excited state properties. Journal of Chemical Physics, 2002, 117, 7433-7447.	1.2	1,992
134	On the density matrix based approach to time-dependent density functional response theory. Journal of Chemical Physics, 2001, 114, 5982-5992.	1.2	385
135	Fullerene C80: Are there still more isomers?. Journal of Chemical Physics, 2001, 114, 10362-10367.	1.2	65
136	Molecular tests of the random phase approximation to the exchange-correlation energy functional. Physical Review B, 2001, 64, .	1.1	400
137	Comment on â€œAssessment of exchange correlation functionalsâ€•[A.J. Cohen, N.C. Handy, Chem. Phys. Lett. 316 (2000) 160â€“166]. Chemical Physics Letters, 2000, 325, 317-321.	1.2	77
138	Structures, Câ€“H and Câ€“CH3 bond energies at borders of polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2000, 2, 5084-5088.	1.3	48
139	Photodissociation spectroscopy of Ag[sub 4][sup +](N[sub 2])[sub m], m=0â€“4. Journal of Chemical Physics, 2000, 113, 5361.	1.2	36
140	Circular Dichroism of Helicenes Investigated by Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2000, 122, 1717-1724.	6.6	470