Michael Dolg

List of Publications by Year
in descending order

251 papers	39,520 citations	15001 68 h-index	3037 194 g-index
286 all docs	286 docs citations	286 times ranked	21888 citing authors

#	Article	IF	Citations
1	Density Functional Studies of Coenzyme NADPH and Its Oxidized Form NADP+: Structures, UVâ€“Vis Spectra, and the Oxidation Mechanism of NADPH. Journal of Computational Chemistry, 2020, 41, 305-316.	1.5	13
2	Structures, electronic properties, hydration and UV-vis absorption spectra of actinide motexafins [An-Motex]2+ (Anâ€‰=â€‰Ac, Cm, Lr) and [UO2-Motex]1+: insights from DFT calculations. Molecular Physics, 2020, 118, e1736676.	0.8	1
3	Periodic trends and complexation chemistry of tetravalent actinide ions with a potential actinide decorporation agent 5â€LIO(Meâ€3,2â€HOPO): A relativistic density functional theory exploration. Journal of Computational Chemistry, 2020, 41, 1427-1435.	1.5	13
4	Enhancing Actinide(III) over Lanthanide(III) Selectivity through Hard-by-Soft Donor Substitution: Exploitation and Implication of Near-Degeneracy-Driven Covalency. Inorganic Chemistry, 2019, 58, 9738-9748.	1.9	34
5	An Efficient Hartreeâ€“Fock Implementation Based on the Contraction of Integrals in the Primitive Basis. Journal of Chemical Theory and Computation, 2018, 14, 6197-6210.	2.3	2
6	Photokatalyse der C(sp³)â€Hâ€Fluorierung durch Uranyl mit sichtbarem Licht: Einblicke in den Mechanismus. Angewandte Chemie, 2018, 130, 11986-11990.	1.6	4
7	The Origin of the Photoluminescence Enhancement of Goldâ€Doped Silver Nanoclusters: The Importance of Relativistic Effects and Heteronuclear Goldâ€“Silver Bonds. Angewandte Chemie - International Edition, 2018, 57, 9965-9969.	7.2	53
8	Ursache der PhotolumineszenzverstÃrkung in Goldâ€dotierten Silberâ€Nanoclustern: BeitrÃge relativistischer Effekte und heteronuklearer Goldâ€Silberâ€Bindungen. Angewandte Chemie, 2018, 130, 10114-10119.	1.6	6
9	Visibleâ€Light Photocatalysis of C(sp³)â€H Fluorination by the Uranyl Ion: Mechanistic Insights. Angewandte Chemie - International Edition, 2018, 57, 11812-11816.	7.2	40
10	Energy Resonance Crossing Controls the Photoluminescence of Europium Antenna Probes. Angewandte Chemie - International Edition, 2017, 56, 7986-7990.	7.2	23
11	The difficult search for organocerium(<scp>iv</scp>) compounds. Chemical Society Reviews, 2017, 46, 6697-6709.	18.7	50
12	The first water coordination sphere of lanthanide(iii) motexafins (Ln-Motex2+, Ln = La, Gd, Lu) and its effects on structures, reduction potentials and UV-vis absorption spectra. Theoretical studies. Physical Chemistry Chemical Physics, 2017, 19, 20160-20171.	1.3	9
13	Energieresonanzkreuzung steuert die Photolumineszenz von Europiumâ€Antennensonden. Angewandte Chemie, 2017, 129, 8097-8101.	1.6	4
14	Relativistic Effective Core Potentials. , 2017, , 449-478.		7
15	Quantum chemical study of the autoxidation of ascorbate. Journal of Computational Chemistry, 2016, 37, 1914-1923.	1.5	4
16	Assigning the Cerium Oxidation State for CH₂CeF₂ and OCeF₂ Based on Multireference Wave Function Analysis. Journal of Physical Chemistry A, 2016, 120, 3966-3974.	1.1	6
17	Global optimization of clusters of rigid molecules using the artificial bee colony algorithm. Physical Chemistry Chemical Physics, 2016, 18, 3003-3010.	1.3	292
18	Regulatory Mechanism of the Enantioselective Intramolecular Enone [2+2] Photocycloaddition Reaction Mediated by a Chiral Lewis Acid Catalyst Containing Heavy Atoms. Angewandte Chemie - International Edition, 2015, 54, 14295-14298.	7.2	35

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19	A theoretical study of imine hydrocyanation catalyzed by halogenâ€bonding. Journal of Computational Chemistry, 2015, 36, 1812-1817.	1.5	9
20	Multi-reference character and Ce 4 f orbital contributions in terminal multiple Ce Z bonds of Cp 2 CeZ (Z = CH 2 , CH â˜ , NH, O, F +) complexes. Computational and Theoretical Chemistry, 2015, 1073, 34-44.	1.1	4
21	Labile Capping Bonds in Lanthanide(III) Complexes: Shorter and Weaker. Journal of Physical Chemistry A, 2015, 119, 774-780.	1.1	17
22	Third-Order Incremental Dual-Basis Set Zero-Buffer Approach for Large High-Spin Open-Shell Systems. Journal of Chemical Theory and Computation, 2015, 11, 962-968.	2.3	10
23	Cerium oxidation state and covalent 4f-orbital contributions in the ground state of bis(Î·8-pentalene)cerium. Journal of Organometallic Chemistry, 2015, 794, 17-22.	0.8	16
24	Accurate quantum chemical modelling of the separation of Eu³⁺from Am³⁺/Cm³⁺by liquidâ€“liquid extraction with Cyanex272. Physical Chemistry Chemical Physics, 2015, 17, 20605-20616.	1.3	41
25	ABCluster: the artificial bee colony algorithm for cluster global optimization. Physical Chemistry Chemical Physics, 2015, 17, 24173-24181.	1.3	415
26	Relativistic Effective Core Potentials. , 2015, , 1-30.		1
27	Approaching the complete basis set limit of CCSD(T) for large systems by the third-order incremental dual-basis set zero-buffer F12 method. Journal of Chemical Physics, 2014, 140, 044114.	1.2	12
28	Coupled-cluster and DFT studies of the Copernicium dimer including QED effects. Chemical Physics Letters, 2014, 616-617, 222-225.	1.2	10
29	Actinoid(III) Hydrationâ€”First Principle Gibbs Energies of Hydration Using High Level Correlation Methods. Journal of Chemical Theory and Computation, 2014, 10, 5593-5598.	2.3	30
30	Relativistic Small-Core Pseudopotentials for Actinium, Thorium, and Protactinium. Journal of Physical Chemistry A, 2014, 118, 2519-2530.	1.1	60
31	Dispersion Interaction Stabilizes Sterically Hindered Double Fullerenes. Chemistry - A European Journal, 2014, 20, 13909-13912.	1.7	21
32	Misleading evidence for covalent bonding from EuIIIX and AmIIIX density functional theory bond lengths. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 8-13.	0.8	26
33	Two interpretations of the cerocene electronic ground state. Chemical Physics Letters, 2014, 594, 47-50.	1.2	46
34	Understanding Lanthanoid(III) Hydration Structure and Kinetics by Insights from Energies and Wave functions. Inorganic Chemistry, 2014, 53, 7700-7708.	1.9	82
35	Third-Order Incremental Dual-Basis Set Zero-Buffer Approach: An Accurate and Efficient Way To Obtain CCSD and CCSD(T) Energies. Journal of Chemical Theory and Computation, 2013, 9, 2992-3003.	2.3	29
36	Accuracy of relativistic energy-consistent pseudopotentials for superheavy elements 111â€“118: Molecular calibration calculations. Journal of Chemical Physics, 2013, 138, 044104.	1.2	22

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37	Relativistic energy-consistent pseudopotentials for superheavy elements 119 and 120 including quantum electrodynamic effects. Journal of Chemical Physics, 2013, 138, 174113.	1.2	20
38	Photoinduced Gold(I)â€“Gold(I) Chemical Bonding in Dicyanoaurate Oligomers. Angewandte Chemie, 2013, 125, 10471-10475.	1.6	8
39	Photoinduced Gold(I)â€“Gold(I) Chemical Bonding in Dicyanoaurate Oligomers. Angewandte Chemie - International Edition, 2013, 52, 10281-10285.	7.2	39
40	Accurate relativistic energy-consistent pseudopotentials for the superheavy elements 111 to 118 including quantum electrodynamic effects. Journal of Chemical Physics, 2012, 136, 214105.	1.2	53
41	Existence of triply charged actinide-hydride molecules. Physical Review A, 2012, 85, .	1.0	10
42	Efficient quantum chemical valence-only treatments of lanthanide and actinide systems. , 2012, , .		2
43	Relativistic Pseudopotentials: Their Development and Scope of Applications. Chemical Reviews, 2012, 112, 403-480.	23.0	346
44	Syntheses, Crystal Structures and Thermal Behavior of Five New Complexes Containing 2, 4, 6â€Trifluorobenzoate as Ligand. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1424-1431.	0.6	14
45	Scalar-relativistic 5f-in-core pseudopotentials and core-polarization potentials for trivalent actinides: calibration calculations for Ac3+, Cm3+ and Lr3+ complexes. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	1
46	Radical 4â€‹exo Cyclizations via Template Catalysis. Chemistry - A European Journal, 2012, 18, 2591-2599.	1.7	25
47	Segmented Contracted Douglasâ€“Krollâ€“Hess Adapted Basis Sets for Lanthanides. Journal of Chemical Theory and Computation, 2011, 7, 3131-3142.	2.3	38
48	Theoretical investigation of thermally and photochemically induced haptotropic rearrangements of chromium ligands on naphthalene systems. Journal of Organometallic Chemistry, 2011, 696, 3861-3866.	0.8	8
49	Pseudopotentials and modelpotentials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 200-210.	6.2	37
50	Improved valence basis sets for divalent lanthanide 4f-in-core pseudopotentials. Theoretical Chemistry Accounts, 2011, 129, 367-379.	0.5	9
51	Localization scheme for relativistic spinors. Journal of Chemical Physics, 2011, 135, 244101.	1.2	6
52	On basis set superposition error corrected stabilization energies for large n-body clusters. Journal of Chemical Physics, 2011, 135, 134118.	1.2	9
53	Fully Automated Implementation of the Incremental Scheme for Correlation Energies. Zeitschrift Fur Physikalische Chemie, 2010, 224, 513-525.	1.4	21
54	Quasirelativistic f-in-core pseudopotentials and core-polarization potentials for trivalent actinides and lanthanides: molecular test for trifluorides. Theoretical Chemistry Accounts, 2010, 126, 117-127.	0.5	87

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55	Fully automated incremental evaluation of MP2 and CCSD(T) core, core-valence and valence correlation energies. Chemical Physics, 2010, 376, 36-45.	0.9	11
56	Combined Computational and Experimental Study of Uranyl(VI) 1:2 Complexation by Aromatic Acids. Inorganic Chemistry, 2010, 49, 6428-6435.	1.9	7
57	First-Principles Study of the Separation of Am^{III}/Cm^{III} from Eu^{III} with Cyanex301. Inorganic Chemistry, 2010, 49, 10307-10315.	1.9	119
58	Computational study of lanthanide(iii) hydration. Physical Chemistry Chemical Physics, 2010, 12, 13215.	1.3	96
59	Automated incremental scheme for explicitly correlated methods. Journal of Chemical Physics, 2010, 132, 164114.	1.2	37
60	Relativistic Pseudopotentials. Challenges and Advances in Computational Chemistry and Physics, 2010, , 215-277.	0.6	23
61	Fully Automated Implementation of the Incremental Scheme for Correlation Energies. , 2010, , 223-235.		0
62	Implementation of the incremental scheme for one-electron first-order properties in coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 154102.	1.2	37
63	A New 5,5â€²-Bitetrazole Thorium(IV) Compound: Synthesis, Crystal Structure and Quantum Chemical Investigation. European Journal of Inorganic Chemistry, 2009, 2009, 2472-2476.	1.0	8
64	On the incremental evaluation of BSSE-free interaction energies. Chemical Physics, 2009, 365, 38-43.	0.9	17
65	Quasirelativistic energy-consistent 4f-in-core pseudopotentials for tetravalent lanthanide elements. Theoretical Chemistry Accounts, 2009, 122, 23-29.	0.5	44
66	Haptotropic migration of M(CO)3 (M=Cr, Mo, W) on substituted phenanthrene. Journal of Organometallic Chemistry, 2009, 694, 3338-3342.	0.8	13
67	Evaluation of core and coreâ€“valence correlation contributions using the incremental scheme. Chemical Physics, 2009, 356, 47-53.	0.9	20
68	Fully Automated Incremental Evaluation of MP2 and CCSD(T) Energies: Application to Water Clusters. Journal of Chemical Theory and Computation, 2009, 5, 287-294.	2.3	109
69	Accurate Relativistic Small-Core Pseudopotentials for Actinides. Energy Adjustment for Uranium and First Applications to Uranium Hydride. Journal of Physical Chemistry A, 2009, 113, 12573-12581.	1.1	96
70	Multiconfiguration Diracâ^'Hartreeâ^'Fock Adjusted Energy-Consistent Pseudopotential for Uranium: Spinâ^'Orbit Configuration Interaction and Fock-Space Coupled-Cluster Study of U⁴⁺ and U⁵⁺. Journal of Physical Chemistry A, 2009, 113, 11509-11516.	1.1	20
71	Energy-consistent pseudopotentials and correlation consistent basis sets for the 5d elements Hfâ€“Pt. Journal of Chemical Physics, 2009, 130, 164108.	1.2	579
72	P-Coligand Tuning of the Haptotropic Metal Migration in Phenanthrene Chromium Complexes. Organometallics, 2009, 28, 3473-3484.	1.1	16

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73	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for pentavalent and hexavalent actinide elements. Theoretical Chemistry Accounts, 2008, 121, 297-306.	0.5	26
74	All-electron Douglasâ€“Krollâ€“Hess and pseudopotential study on the low-lying states of uranium hydride UH. Chemical Physics, 2008, 343, 250-257.	0.9	17
75	Using symmetry in the framework of the incremental scheme: Molecular applications. Chemical Physics, 2008, 346, 266-274.	0.9	28
76	On the performance of two-component energy-consistent pseudopotentials in atomic Fock-space coupled cluster calculations. Journal of Chemical Physics, 2008, 128, 024106.	1.2	15
77	Complexation of Uranium(VI) with Aromatic Acids in Aqueous Solution: A Combined Computational and Experimental Study. Inorganic Chemistry, 2008, 47, 3150-3157.	1.9	17
78	Energy-consistent small-core pseudopotentials for 3d-transition metals adapted to quantum Monte Carlo calculations. Journal of Chemical Physics, 2008, 129, 164115.	1.2	102
79	Evaluation of Incremental Correlation Energies for Open-Shell Systems: Application to the Intermediates of the 4-Exo Cyclization, Arduengo Carbenes and an Anionic Water Cluster. Journal of Physical Chemistry A, 2008, 112, 8762-8766.	1.1	31
80	Implementation and performance of a domain-specific basis set incremental approach for correlation energies: Applications to hydrocarbons and a glycine oligomer. Journal of Chemical Physics, 2008, 129, 244105.	1.2	57
81	Titanocene Catalyzed 4-exoCyclizations:Â Mechanism, Experiment, Catalyst Design. Journal of the American Chemical Society, 2008, 130, 1788-1796.	6.6	72
82	Fully automated implementation of the incremental scheme: Application to CCSD energies for hydrocarbons and transition metal compounds. Journal of Chemical Physics, 2007, 126, 154110.	1.2	154
83	Evaluation of electronic correlation contributions for optical tensors of large systems using the incremental scheme. Journal of Chemical Physics, 2007, 127, 084108.	1.2	12
84	Energy-consistent relativistic pseudopotentials and correlation consistent basis sets for the 4d elements Yâ€“Pd. Journal of Chemical Physics, 2007, 126, 124101.	1.2	822
85	Approaching actinide(+III) hydration from first principles. Physical Chemistry Chemical Physics, 2007, 9, 459-465.	1.3	94
86	A Quantum Chemical Study of the Haptotropic Rearrangements of Cr(CO)3on Naphthalene and Phenanthrene Systems. Journal of Physical Chemistry A, 2007, 111, 6094-6102.	1.1	35
87	Energy Screening for the Incremental Scheme:â€‰ Application to Intermolecular Interactions. Journal of Physical Chemistry A, 2007, 111, 9830-9837.	1.1	45
88	Computational investigation of the Bi lone-pairs in monoclinic bismuth triborate BiB3O6. Physical Chemistry Chemical Physics, 2007, 9, 2094.	1.3	20
89	First-principles calculation of vibrational frequencies for monoclinic tribismuth borate BiB3O6. Zeitschrift FÃ¼r Kristallographie, 2007, 222, .	1.1	2
90	Energy-consistent pseudopotentials for quantum Monte Carlo calculations. Journal of Chemical Physics, 2007, 126, 234105.	1.2	305

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91	Error analysis of incremental electron correlation calculations and applications to clusters and potential energy surfaces. Chemical Physics, 2007, 338, 33-43.	0.9	34
92	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for trivalent actinide elements. Theoretical Chemistry Accounts, 2007, 117, 473-481.	0.5	88
93	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for divalent and tetravalent actinide elements. Theoretical Chemistry Accounts, 2007, 118, 845-854.	0.5	78
94	The performance of the Hartreeâ€“Fockâ€“Wigner correlation model for light diatomic molecules. Theoretical Chemistry Accounts, 2007, 118, 777-783.	0.5	4
95	Quasirelativistic 5f-in-core pseudopotential study of the actinocenes An(C8H8)2, An=Thâ€“Pu. Chemical Physics, 2007, 337, 48-54.	0.9	19
96	Phase stabilities of monoclinic oxoborates LaB3O6 and GdB3O6 in C121 and I12/a1 phaseâ€”Energetics and chemical bonds derived from first-principles calculations. Journal of Solid State Chemistry, 2007, 180, 2763-2774.	1.4	3
97	First-Principles Electronic Structure Study of the Monoclinic Crystal Bismuth Triborate BiB3O6. Journal of Physical Chemistry B, 2006, 110, 19254-19263.	1.2	38
98	Density Functional Theory Studies of Actinide(III) Motexafins (An-Motex2+, An = Ac, Cm, Lr). Structure, Stability, and Comparison with Lanthanide(III) Motexafins. Inorganic Chemistry, 2006, 45, 3444-3451.	1.9	30
99	Relativistic energy-consistent ab initio pseudopotentials as tools for quantum chemical investigations of actinide systems. Coordination Chemistry Reviews, 2006, 250, 900-910.	9.5	66
100	A quantum chemical ab initio study of the polymerization to polyhydridophosphazenes. Chemical Physics, 2006, 325, 291-298.	0.9	4
101	A PH-Functionalized Polyphosphazene: A Macromolecule with a Highly Flexible Backbone. Angewandte Chemie - International Edition, 2006, 45, 3083-3086.	7.2	14
102	Energy-consistent pseudopotentials for group 11 and 12 atoms: adjustment to multi-configuration Diracâ€“Hartreeâ€“Fock data. Chemical Physics, 2005, 311, 227-244.	0.9	854
103	Molecular results for the Hartreeâ€“Fockâ€“Wigner model. Chemical Physics Letters, 2005, 413, 237-241.	1.2	6
104	Valence basis sets for lanthanide 4f-in-core pseudopotentials adapted for crystal orbital ab initio calculations. Theoretical Chemistry Accounts, 2005, 113, 212-224.	0.5	121
105	Improved relativistic energy-consistent pseudopotentials for 3d-transition metals. Theoretical Chemistry Accounts, 2005, 114, 297-304.	0.5	39
106	Hermann Stoll. Theoretical Chemistry Accounts, 2005, 114, 253-254.	0.5	0
107	PSEUDOPOTENTIAL STUDIES ON THE ELECTRONIC STRUCTURE OF LANTHANUM MONOHALIDES LaF, LaCl, LaBr, AND LaI. Journal of Theoretical and Computational Chemistry, 2005, 04, 583-592.	1.8	12
108	Bent and planar molecules in polymorphs of the tricyclic carbon sulfide C6S8. New Journal of Chemistry, 2005, 29, 465.	1.4	13

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109	A Combined Theoretical and Experimental Study of Efficient and Fast Titanocene-Catalyzed3-exoCyclizations. Journal of the American Chemical Society, 2005, 127, 7071-7077.	6.6	73
110	Haptotropic Metal Migration in Densely Substituted Hydroquinoid Phenanthrene Cr(CO)3 Complexes1. Organometallics, 2005, 24, 3219-3228.	1.1	46
111	Static and dynamic properties of amorphous material derived from zeolite ZSM-5. Journal of Non-Crystalline Solids, 2005, 351, 1151-1157.	1.5	3
112	Ab initio many-body investigation of structure and stability of two-fold rings in silicates. Journal of Chemical Physics, 2004, 120, 8734-8739.	1.2	12
113	Low-frequency vibrational excitations in zeolite ZSM-5 and its partially crystalline derivatives. Physical Review B, 2004, 69, .	1.1	11
114	THE RELATIVISTIC ENERGY-CONSISTENT AB INITIO PSEUDOPOTENTIAL APPROACH AND ITS APPLICATION TO LANTHANIDE AND ACTINIDE COMPOUNDS. Recent Advances in Computational, 2004, , 1-35.	0.8	16
115	Segmented contraction scheme for small-core actinide pseudopotential basis sets. Computational and Theoretical Chemistry, 2004, 673, 203-209.	1.5	616
116	Molecular Dynamics Investigation of Relaxations in Zeolite ZSM-5 Based Amorphous Material. Journal of Physical Chemistry B, 2004, 108, 16085-16092.	1.2	3
117	Electron affinity of Ce and electronic states ofCeâ^'. Physical Review A, 2004, 69, .	1.0	18
118	Systematically convergent basis sets with relativistic pseudopotentials. II. Small-core pseudopotentials and correlation consistent basis sets for the post-d group 16â€“18 elements. Journal of Chemical Physics, 2003, 119, 11113-11123.	1.2	1,855
119	Valence basis sets for relativistic energy-consistent small-core actinide pseudopotentials. Journal of Chemical Physics, 2003, 118, 487-496.	1.2	640
120	Density functional studies on lanthanide (III) texaphyrins (Ln-Tex2+, Ln = La, Gd, Lu): structure, stability and electronic excitation spectrum. Molecular Physics, 2003, 101, 2427-2435.	0.8	26
121	Theoretical prediction of the second to fourth actinide ionization potentials. Molecular Physics, 2003, 101, 961-969.	0.8	54
122	Electronic structure of lanthanide dimers. Molecular Physics, 2003, 101, 1967-1976.	0.8	44
123	Molecular dynamics investigation of vibrational properties of zeolite ZSM-5-based amorphous material. Physical Review B, 2003, 68, .	1.1	11
124	Molecular dynamics investigation of structural properties of a zeolite ZSM-5 based amorphous material. Physical Review B, 2003, 67, .	1.1	12
125	Calibration of Relativistic Energyâ€Consistent Smallâ€Core Pseudopotentials for 3dâ€Transition Metals. Journal of the Chinese Chemical Society, 2003, 50, 583-592.	0.8	4
126	Ab initiomany-body calculations on infinite carbon and boron-nitrogen chains. Physical Review B, 2002, 65, .	1.1	73

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127	QUANTUM MONTE CARLO STUDY OF MERCURY CLUSTERS. Recent Advances in Computational, 2002, , 183-202.	0.8	0
128	Molecular structure of diatomic lanthanide compounds. Science in China Series B: Chemistry, 2002, 45, 91.	0.8	37
129	Relativistic energy-consistent pseudopotentials?Recent developments. Journal of Computational Chemistry, 2002, 23, 767-778.	1.5	221
130	Pseudopotential study of lanthanum and lutetium dimers. Theoretical Chemistry Accounts, 2002, 108, 143-149.	0.5	43
131	Segmented contraction scheme for small-core lanthanide pseudopotential basis sets. Computational and Theoretical Chemistry, 2002, 581, 139-147.	1.5	653
132	Electron correlation effects on structural and cohesive properties of closo-hydroborate dianions (BnHn)2- (n = 5â€“12) and B4H4. Physical Chemistry Chemical Physics, 2001, 3, 514-522.	1.3	30
133	Valence basis sets for relativistic energy-consistent small-core lanthanide pseudopotentials. Journal of Chemical Physics, 2001, 115, 7348-7355.	1.2	574
134	Combined Pseudopotential and Density Functional Study of Bis-Î·6-benzene d and f Element Complexes. Journal of Chemical Information and Computer Sciences, 2001, 41, 18-21.	2.8	30
135	Structures of mercury clusters in a quantumâ€“empirical hybrid model. Physical Chemistry Chemical Physics, 2001, 3, 5121-5129.	1.3	31
136	Theoretische Chemie 2000. Nachrichten Aus Der Chemie, 2001, 49, 337-345.	0.0	0
137	Bi4Te44+â€”A Cube-Shaped, Polycationic Main Group Element Cluster. Angewandte Chemie - International Edition, 2001, 40, 2287-2290.	7.2	50
138	On the performance of energy-consistent spinâ€“orbit pseudopotentials: (111)H revisited. Chemical Physics Letters, 2001, 345, 490-496.	1.2	24
139	Basis set limit extrapolation of ACPF and CCSD(T) results for the third and fourth lanthanide ionization potentials. Chemical Physics Letters, 2001, 349, 489-495.	1.2	28
140	A comparison of scalar-relativistic ZORA and DKH density functional schemes: monohydrides, monooxides and monofluorides of La, Lu, Ac and Lr. Chemical Physics Letters, 2001, 334, 396-402.	1.2	67
141	Bi(4)Te(4)(4+)-A Cube-Shaped, Polycationic Main Group Element Cluster This work was supported by the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie.. Angewandte Chemie - International Edition, 2001, 40, 2287-2290.	7.2	0
142	Performance of relativistic density functional and ab initio pseudopotential approaches for systems with high-spin multiplicities: Gadolinium diatomics GdX (X=H, N, O, F, P, S, Cl, Gd). International Journal of Quantum Chemistry, 2000, 76, 359-370.	1.0	72
143	Scalar-relativistic density functional and ab initio pseudopotential study of zero-valentd andf metal bis-?6-benzene sandwich complexes M(C6H6)2 (M = Sc, Ti, Y, Zr, La, Lu, Hf, Th, U). International Journal of Quantum Chemistry, 2000, 80, 201-209.	1.0	31
144	Structural changes induced by an excess electron in small mercury clusters. International Journal of Mass Spectrometry, 2000, 201, 197-204.	0.7	14

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145	Correlated ground-state ab initio calculations of polymethineimine. Chemical Physics, 2000, 257, 301-310.	0.9	13
146	A small-core multiconfiguration Dirac-Hartree-Fock-adjusted pseudopotential for Tl - application to Tl X (X = F, Cl, Br, I). Theoretical Chemistry Accounts, 2000, 104, 22-28.	0.5	138
147	Realistic hybrid model for correlation effects in mercury clusters. Physical Review B, 2000, 61, 2362-2370.	1.1	23
148	Ab initiotreatment of electron correlations in polymers: Lithium hydride chain and beryllium hydride polymer. Journal of Chemical Physics, 2000, 112, 4801-4805.	1.2	40
149	Small-core multiconfiguration-Diracâ€“Hartreeâ€“Fock-adjusted pseudopotentials for post-d main group elements: Application to PbH and PbO. Journal of Chemical Physics, 2000, 113, 2563-2569.	1.2	1,009
150	Ab Initio Study of Structure and Bonding of Strontium Clusters. Journal of Physical Chemistry A, 2000, 104, 5558-5567.	1.1	28
151	Ab initio study of structural and cohesive properties of polymers: Polyiminoborane and polyaminoborane. Journal of Chemical Physics, 1999, 110, 8819-8824.	1.2	46
152	Wave-function-based correlatedab initiocalculations on crystalline solids. Physical Review B, 1999, 60, 5211-5216.	1.1	73
153	Theoretical confirmation of the stereoselectivity in the reverse Brook rearrangement. Tetrahedron, 1999, 55, 12751-12756.	1.0	26
154	Relativistic ab initio and density functional theory calculations on the mercury fluorides: Is HgF4 thermodynamically stable?. Chemical Physics Letters, 1999, 302, 231-239.	1.2	40
155	On the Importance of 5d Orbitals for Covalent Bonding in Ytterbium Clusters. Journal of Physical Chemistry A, 1999, 103, 5091-5098.	1.1	10
156	Ab Initio Study of the Reaction Mechanism of CH3+ and CH3- with CH2CNa(OH). Journal of Physical Chemistry A, 1999, 103, 3472-3480.	1.1	0
157	Ab Initio Study of Metalâ^'Ring Bonding in the Bis(Î·6-benzene)lanthanide and -actinide Complexes M(C6H6)2(M = La, Ce, Nd, Gd, Tb, Lu, Th, U). Journal of the American Chemical Society, 1999, 121, 1502-1512.	6.6	59
158	A Hartreeâ€“Fock ab initio band-structure calculation employing Wannier-type orbitals. Chemical Physics Letters, 1998, 285, 174-179.	1.2	17
159	A Wannier-function-based ab initio Hartreeâ€“Fock study of polyethylene. Chemical Physics Letters, 1998, 294, 126-134.	1.2	8
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