H Georg Schreckenbach

List of Publications by Year
in descending order

126 papers	8,068 citations	66234 42 h-index	49773 87 g-index
131 all docs	131 docs citations	131 times ranked	6377 citing authors

#	Article	IF	Citations
1	Actinium coordination chemistry: A density functional theory study with monodentate and bidentate ligands. Journal of Computational Chemistry, 2023, 44, 334-345.	1.5	1
2	Achieved negative differential resistance behavior of Si/B-substituted into a C6 chain sandwiched between capped carbon nanotube junctions. RSC Advances, 2022, 12, 1758-1768.	1.7	0
3	Methods for Interpreting the Partitioning and Fate of Petroleum Hydrocarbons in a Sea Ice Environment. Journal of Physical Chemistry A, 2022, 126, 772-786.	1.1	3
4	Prediction of beryllium clusters (Be_n; n = 3â€“25) from first principles. Physical Chemistry Chemical Physics, 2021, 23, 19716-19728.	1.3	15
5	Stabilization of hydrated Ac^{III} cation: the role of superatom states in actinium-water bonding. Chemical Science, 2021, 12, 2655-2666.	3.7	10
6	Computational Characterization of Ac^{III}-DOTA Complexes in Aqueous Solution. Inorganic Chemistry, 2021, 60, 6971-6975.	1.9	5
7	Computational Study of Actinyl Ion Complexation with Dipyriamethyrin Macrocyclic Ligands. Journal of Physical Chemistry A, 2021, 125, 920-932.	1.1	11
8	Theoretical Study of p- and n-Doping of Polythiophene- and Polypyrrole-Based Conjugated Polymers. Journal of Physical Chemistry C, 2020, 124, 17528-17537.	1.5	16
9	Ab initio study of strain and electric field dependent variation in electronic and thermoelectric properties of PdS2. Materials Today Communications, 2020, 24, 100976.	0.9	12
10	Interaction potential energy surface between superatoms. Chemical Communications, 2020, 56, 14681-14684.	2.2	10
11	Dielsâ€“Alder reaction of tetraarylcyclopentadienones with benzo[b]thiophene S,S-dioxides: an unprecedented de-oxygenation vs. sulfur dioxide extrusion. Chemical Communications, 2020, 56, 15317-15320.	2.2	9
12	Proton affinities of pertechnetate (TcO_4^-) and perrhenate (ReO_4^-). Physical Chemistry Chemical Physics, 2020, 22, 12403-12411.	1.3	2
13	Adsorption of Actinide (Uâ€“Pu) Complexes on the Silicene and Germanene Surface: A Theoretical Study. Journal of Physical Chemistry A, 2020, 124, 1522-1534.	1.1	3
14	Differential uranyl(v) oxo-group bonding between the uranium and metal cations from groups 1, 2, 4, and 12; a high energy resolution X-ray absorption, computational, and synthetic study. Chemical Science, 2019, 10, 9740-9751.	3.7	29
15	Theoretical investigation of U(<scp>i</scp>) arene complexes: is the elusive monovalent oxidation state accessible?. New Journal of Chemistry, 2019, 43, 1469-1477.	1.4	13
16	Environmental Mercury Chemistry â€“ In Silico. Accounts of Chemical Research, 2019, 52, 379-388.	7.6	40
17	Interdisciplinary Round-Robin Test on Molecular Spectroscopy of the U(VI) Acetate System. ACS Omega, 2019, 4, 8167-8177.	1.6	5
18	Could new U(ii) complexes be accessible via tuning hybrid heterocalix[4]arene? A theoretical study of redox and structural properties. Dalton Transactions, 2018, 47, 2148-2151.	1.6	11

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19	Molecular Recognition of Hydrophilic Molecules in Water by Combining the Hydrophobic Effect with Hydrogen Bonding. Journal of the American Chemical Society, 2018, 140, 13466-13477.	6.6	130
20	Simple computational screening of potential singlet fission molecules. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	5
21	Interfacial Interaction of Titania Nanoparticles and Ligated Uranyl Species: A Relativistic DFT Investigation. Inorganic Chemistry, 2017, 56, 2763-2776.	1.9	11
22	Differential Solvation. Chemistry - A European Journal, 2017, 23, 3797-3803.	1.7	20
23	Frontispiece: Differential Solvation. Chemistry - A European Journal, 2017, 23, .	1.7	1
24	Polythiophene: From Fundamental Perspectives to Applications. Chemistry of Materials, 2017, 29, 10248-10283.	3.2	286
25	Relativistic DFT and experimental studies of mono- and bis-actinyl complexes of an expanded Schiff-base polypyrrole macrocycle. Dalton Transactions, 2016, 45, 15910-15921.	1.6	15
26	Theoretical investigation of low-valent uranium and transuranium complexes of a flexible small-cavity macrocycle: structural, formation reaction and redox properties. Dalton Transactions, 2016, 45, 15970-15982.	1.6	18
27	Topological phase in oxidized zigzag stanene nanoribbons. AIP Advances, 2016, 6, 095019.	0.6	8
28	Materials properties of out-of-plane heterostructures of MoS2-WSe2 and WS2-MoSe2. Applied Physics Letters, 2016, 108, .	1.5	79
29	Subtle Interactions and Electron Transfer between U^{III}, Np^{III}, or Pu^{III} and Uranyl Mediated by the Oxo Group. Angewandte Chemie, 2016, 128, 12989-12993.	1.6	15
30	Implementation of the SM12 Solvation Model into ADF and Comparison with COSMO. Journal of Chemical Theory and Computation, 2016, 12, 4033-4041.	2.3	14
31	A computational investigation of polypyrrolic macrocyclic actinyl complexes: effects of explicit solvent coordination on structure, vibrational spectra and redox property. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
32	Subtle Interactions and Electron Transfer between U^{III}, Np^{III}, or Pu^{III} and Uranyl Mediated by the Oxo Group. Angewandte Chemie - International Edition, 2016, 55, 12797-12801.	7.2	40
33	Band gap modulation in polythiophene and polypyrrole-based systems. Scientific Reports, 2016, 6, 36554.	1.6	41
34	Structural and Electronic Properties of Pristine and Doped Polythiophene: Periodic versus Molecular Calculations. Journal of Physical Chemistry C, 2015, 119, 3979-3989.	1.5	39
35	Fluorescence Enhancement/Quenching Based on Metal Orbital Control: Computational Studies of a 6-Thienyllumazine-Based Mercury Sensor. Journal of Physical Chemistry A, 2015, 119, 8106-8116.	1.1	49
36	Electrically Engineered Band Gap in Two-Dimensional Ge, Sn, and Pb: A First-Principles and Tight-Binding Approach. Journal of Physical Chemistry C, 2015, 119, 11896-11902.	1.5	41

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37	Highly Valence-Diversified Binuclear Uranium Complexes of a Schiff-Base Polypyrrolic Macrocycle: Prediction of Unusual Structures, Electronic Properties, and Formation Reactions. Inorganic Chemistry, 2015, 54, 5438-5449.	1.9	17
38	Highly Diverse Bonding between Two U³⁺ Ions When Ligated by a Flexible Polypyrrolic Macrocycle. Organometallics, 2015, 34, 5225-5232.	1.1	22
39	Substitution Effects on the Water Oxidation of Ruthenium Catalysts: A Quantum-Chemical Look. Journal of Physical Chemistry C, 2015, 119, 242-250.	1.5	15
40	Theoretical Study of the Formation of Mercury (Hg²⁺) Complexes in Solution Using an Explicit Solvation Shell in Implicit Solvent Calculations. Journal of Physical Chemistry B, 2014, 118, 11271-11283.	1.2	16
41	Oxo-Exchange of Gas-Phase Uranyl, Neptunyl, and Plutonyl with Water and Methanol. Inorganic Chemistry, 2014, 53, 2163-2170.	1.9	19
42	Large Enhancement and Tunable Band Gap in Silicene by Small Organic Molecule Adsorption. Journal of Physical Chemistry C, 2014, 118, 23361-23367.	1.5	162
43	Conformation/Tautomerization effect on the pK_a values of lumazine and 6â€thienyllumazine. Journal of Physical Organic Chemistry, 2014, 27, 690-700.	0.9	3
44	Investigation of the Electronic Structure of Mono(1,1â€²-Diamidoferrocene) Uranium(IV) Complexes. Organometallics, 2013, 32, 6012-6021.	1.1	27
45	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8
46	Oxo-Functionalization and Reduction of the Uranyl Ion through Lanthanide-Element Bond Homolysis: Synthetic, Structural, and Bonding Analysis of a Series of Singly Reduced Uranylâ€“Rare Earth 5f¹-4fⁿ Complexes. Journal of the American Chemical Society, 2013, 135, 3841-3854.	6.6	107
47	Conformational Preference of Fused Carbohydrate-Templated Proline Analoguesâ€”A Computational Study. Journal of Physical Chemistry B, 2013, 117, 199-205.	1.2	3
48	Theoretical Study of Structural, Spectroscopic and Reaction Properties of trans-bis(imido) Uranium(VI) Complexes. Inorganic Chemistry, 2013, 52, 9143-9152.	1.9	11
49	DFT Study of Uranyl Peroxo Complexes with H₂O, F^{â€“}, OH^{â€“}, CO₃²⁻, and NO₃^{â€“}. Inorganic Chemistry, 2013, 52, 5590-5602.	1.9	40
50	DFT Study of Oxo-Functionalized Pentavalent Dioxouranium Complexes: Structure, Bonding, Ligand Exchange, Dimerization, and U(V)/U(IV) Reduction of OUOH and OUOSiH3Complexes. Inorganic Chemistry, 2013, 52, 245-257.	1.9	8
51	Theoretical exploration of uranyl complexes of a designed polypyrrolic macrocycle: structure/property effects of hinge size on Pacman-shaped complexes. Dalton Transactions, 2012, 41, 8878.	1.6	24
52	Quantum-Chemical Study of the Diffusion of Hg(0, I, II) into the Ice(Ih). Journal of Physical Chemistry C, 2012, 116, 5151-5154.	1.5	10
53	Relationship between dyeâ€“iodine binding and cell voltage in dyeâ€sensitized solar cells: A quantumâ€mechanical look. Journal of Computational Chemistry, 2012, 33, 2492-2497.	1.5	16
54	Pteridine-based fluorescent pH sensors designed for physiological applications. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 247, 63-73.	2.0	14

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55	Strongly coupled binuclear uraniumâ€“oxo complexes from uranyl oxo rearrangement and reductive silylation. Nature Chemistry, 2012, 4, 221-227.	6.6	149
56	Co-linear, double-uranyl coordination by an expanded Schiff-base polypyrrole macrocycle. Dalton Transactions, 2012, 41, 6595.	1.6	28
57	Theoretical Study of the Reduction of Uranium(VI) Aquo Complexes on Titania Particles and by Alcohols. Chemistry - A European Journal, 2012, 18, 7117-7127.	1.7	29
58	Density functional study of substituted (â€“SH, â€“S, â€“OH, â€“Cl) hydrated ions of Hg2+. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	12
59	Adsorption of Uranyl Species onto the Rutile (110) Surface: A Periodic DFT Study. Chemistry - A European Journal, 2012, 18, 1458-1466.	1.7	37
60	Theoretical predictions of cofacial bis(actinyl) complexes of a stretched Schiff-base calixpyrrole ligand. Chemical Communications, 2011, 47, 5720.	2.2	44
61	QM and QM/MM Studies of Uranyl Fluorides in the Gas and Aqueous Phases and in the Hydrophobic Cavities of Tetrabrachion. Inorganic Chemistry, 2011, 50, 3141-3152.	1.9	22
62	Degradation Mechanism of Methyl Mercury Selenoamino Acid Complexes: A Computational Study. Inorganic Chemistry, 2011, 50, 2366-2372.	1.9	41
63	Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colleâ^'Salvetti Correlation Density Functionals.. Journal of Chemical Theory and Computation, 2011, 7, 804-806.	2.3	2
64	Theoretical Study of the Structural Properties of Plutonium(IV) and (VI) Complexes. Journal of Physical Chemistry A, 2011, 115, 14110-14119.	1.1	35
65	Interactions of the N3 dye with the iodide redox shuttle: quantum chemical mechanistic studies of the dye regeneration in the dye-sensitized solar cell. Physical Chemistry Chemical Physics, 2011, 13, 15148.	1.3	28
66	Chalcogenophilicity of Mercury. Inorganic Chemistry, 2011, 50, 3791-3798.	1.9	26
67	Computational studies of the interactions of Iâ^' and I3 â^' with TiO2 clusters: implications for dye-sensitized solar cells. Theoretical Chemistry Accounts, 2011, 129, 199-208.	0.5	14
68	Characterising Loneâ€Pair Activity of Lead(II) by ²⁰⁷Pb Solidâ€State NMR Spectroscopy: Coordination Polymers of [N(CN)₂]^{â^'} and [Au(CN)₂]^{â^'} with Terpyridine Ancillary Ligands. Chemistry - A European Journal, 2011, 17, 3609-3618.	1.7	49
69	Performance of Relativistic Effective Core Potentials in DFT Calculations on Actinide Compounds. Journal of Physical Chemistry A, 2010, 114, 1957-1963.	1.1	60
70	Binuclear Uranium(VI) Complexes with a â€œPacmanâ€•Expanded Porphyrin: Computational Evidence for Highly Unusual Bisâ€Actinyl Structures. Chemistry - A European Journal, 2010, 16, 2282-2290.	1.7	45
71	Computational Studies of the Interaction between Ruthenium Dyes and Xâ^' and X2â^', X = Br, I, At. Implications for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 15165-15173.	1.5	25
72	Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colleâ^'Salvetti Correlation Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 3442-3455.	2.3	16

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73	Binuclear Hexa- and Pentavalent Uranium Complexes with a Polypyrrolic Ligand: A Density Functional Study of Water- and Hydronium-Induced Reactions. Inorganic Chemistry, 2010, 49, 6509-6517.	1.9	44
74	Oxygen Exchange in Uranyl Hydroxide via Two â€œNonclassicalâ€•Ions. Inorganic Chemistry, 2010, 49, 3821-3827.	1.9	48
75	Computational Studies of Structural, Electronic, Spectroscopic, and Thermodynamic Properties of Methylmercury-Amino Acid Complexes and Their Se Analogues. Inorganic Chemistry, 2010, 49, 870-878.	1.9	24
76	Theoretical Actinide Molecular Science. Accounts of Chemical Research, 2010, 43, 19-29.	7.6	210
77	Performance of the Empirical Dispersion Corrections to Density Functional Theory: Thermodynamics of Hydrocarbon Isomerizations and Olefin Monomer Insertion Reactions. Journal of Chemical Theory and Computation, 2010, 6, 477-490.	2.3	44
78	Adsorption of Na and Hg on the Ice(Ih) Surface: A Density-Functional Study. Journal of Physical Chemistry C, 2010, 114, 2941-2946.	1.5	6
79	Computational studies on the interactions among redox couples, additives and TiO2: implications for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2010, 12, 14609.	1.3	32
80	Computational study of the ground state properties of iodine and polyiodide ions. Theoretical Chemistry Accounts, 2009, 122, 119-125.	0.5	32
81	Effect of Counterions on the Structure and Stability of Aqueous Uranyl(VI) Complexes. A First-Principles Molecular Dynamics Study. Inorganic Chemistry, 2009, 48, 9977-9979.	1.9	25
82	Intramolecular Hydrogen Bond-Controlled Prolyl Amide Isomerization in Glucosyl 3â€²(S)-Hydroxy-5â€²-hydroxymethylproline Hybrids: Influence of a C-5â€²-Hydroxymethyl Substituent on the Thermodynamics and Kinetics of Prolyl Amide Cis/Trans Isomerization. Journal of Organic Chemistry, 2009, 74, 3735-3743.	1.7	19
83	Synthesis, characterization and structures of methylmercury complexes with selenoamino acids. Dalton Transactions, 2009, , 5766.	1.6	27
84	Neptunium(VII) in high-ionic-strength alkaline solutions â€” [NpO₂(OH)₄]^{1â€“} or [NpO₄(OH)₂]^{3â€“}?. Canadian Journal of Chemistry, 2009, 87, 1436-1443.	0.6	9
85	Crown Ether Inclusion Complexes of the Early Actinide Elements, [AnO₂(18-crown-6)]ⁿ⁺, An = U, Np, Pu andn= 1, 2: A Relativistic Density Functional Study. Inorganic Chemistry, 2008, 47, 1465-1475.	1.9	117
86	Theoretical Study of the Oxygen Exchange in Uranyl Hydroxide. An Old Riddle Solved?. Journal of the American Chemical Society, 2008, 130, 13735-13744.	6.6	61
87	Computational Density Functional Study of Polypyrrolic Macrocycles: Analysis of Actinyl-Oxo to 3d Transition Metal Bonding. Inorganic Chemistry, 2008, 47, 11583-11592.	1.9	35
88	The Role of Peripheral Alkyl Substituents:â€‰ A Theoretical Study of Substituted and Unsubstituted Uranyl Isoamethyrin Complexes. Inorganic Chemistry, 2008, 47, 805-811.	1.9	24
89	Structural and Spectroscopic Impact of Tuning the Stereochemical Activity of the Lone Pair in Lead(II) Cyanoaurate Coordination Polymers via Ancillary Ligands. Inorganic Chemistry, 2008, 47, 6353-6363.	1.9	50
90	Density Functional Study of Lithium Hexamethyldisilazide (LiHMDS) Complexes:Â Effects of Solvation and Aggregation. Inorganic Chemistry, 2007, 46, 3856-3864.	1.9	17

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91	A Density Functional Study of the Various Forms of UN4O12Containing Uranyl Nitrate. Journal of Physical Chemistry A, 2007, 111, 10789-10803.	1.1	8
92	A Comparative Relativistic DFT and Ab Initio Study on the Structure and Thermodynamics of the Oxofluorides of Uranium(IV), (V) and (VI). Chemistry - A European Journal, 2007, 13, 4932-4947.	1.7	142
93	Relativistic Density Functional Theory Study of Dioxoactinide(VI) and -(V) Complexation with Alaskaphyrin and Related Schiff-Base Macrocyclic Ligands. Journal of Physical Chemistry A, 2006, 110, 9486-9499.	1.1	72
94	Density Functional Studies of Actinyl Aquo Complexes Studied Using Small-Core Effective Core Potentials and a Scalar Four-Component Relativistic Method. Journal of Physical Chemistry A, 2005, 109, 10961-10974.	1.1	218
95	Density functional calculations of 19 F and 235 U NMR chemical shifts in uranium (VI) chloride fluorides UF6âˆ'n Cl n : Influence of the relativistic approximation and role of the exchange-correlation functional. International Journal of Quantum Chemistry, 2005, 101, 372-380.	1.0	31
96	Calculation of EPR g-Tensors with Density Functional Theory. , 2004, , 505-532.		24
97	NMR quantum computing: applying theoretical methods to designing enhanced systems. Magnetic Resonance in Chemistry, 2004, 42, S88-S98.	1.1	12
98	QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis. Computational and Theoretical Chemistry, 2003, 632, 1-28.	1.5	887
99	NMR Shielding Calculations across the Periodic Table:Â Diamagnetic Uranium Compounds. 2. Ligand and Metal NMR. Inorganic Chemistry, 2002, 41, 6560-6572.	1.9	33
100	On the relation between a common gauge origin formulation and the GIAO formulation of the NMR shielding tensor. Theoretical Chemistry Accounts, 2002, 108, 246-253.	0.5	25
101	Mixed Uranium Chloride Fluorides UF6-nClnand Methoxyuranium Fluorides UF6-n(OCH3)n:Â A Theoretical Study of Equilibrium Geometries, Vibrational Frequencies, and the Role of the f Orbitals. Inorganic Chemistry, 2000, 39, 1265-1274.	1.9	28
102	NMR Shielding Calculations across the Periodic Table:â€‰ Diamagnetic Uranium Compounds. 1. Methods and Issues. Journal of Physical Chemistry A, 2000, 104, 8244-8255.	1.1	66
103	Relativistic Effects for NMR Shielding Constants in Transition Metal Oxides Using the Zeroth-Order Regular Approximation. Journal of Physical Chemistry A, 2000, 104, 5600-5611.	1.1	70
104	Theoretical Studies of the Properties and Solution Chemistry of AnO22+and AnO2+Aquo Complexes for An = U, Np, and Pu. Journal of Physical Chemistry A, 2000, 104, 6259-6270.	1.1	260
105	Density functional calculations on actinide compounds: Survey of recent progress and application to [UO2X4]2? (X=F, Cl, OH) and AnF6 (An=U, Np, Pu). Journal of Computational Chemistry, 1999, 20, 70-90.	1.5	230
106	The 57Fe nuclear magnetic resonance shielding in ferrocene revisited. A density-functional study of orbital energies, shielding mechanisms, and the influence of the exchange-correlation functional. Journal of Chemical Physics, 1999, 110, 11936-11949.	1.2	79
107	Covering the Entire Periodic Table: Relativistic Density Functional Calculations of NMR Chemical Shifts in Diamagnetic Actinide Compounds. ACS Symposium Series, 1999, , 101-114.	0.5	6
108	Density functional calculations of NMR chemical shifts and ESR g-tensors. Theoretical Chemistry Accounts, 1998, 99, 71-82.	0.5	215

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109	Theoretical Study of Stable Trans and Cis Isomers in [UO2(OH)4]2-Using Relativistic Density Functional Theory. Inorganic Chemistry, 1998, 37, 4442-4451.	1.9	137
110	Calculation of125Te Chemical Shifts Using Gauge-Including Atomic Orbitals and Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 4121-4127.	1.1	48
111	Calculation of the G-Tensor of Electron Paramagnetic Resonance Spectroscopy Using Gauge-Including Atomic Orbitals and Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 3388-3399.	1.1	244
112	Calculation of NMR shielding tensors based on density functional theory and a scalar relativistic Pauli-type Hamiltonian. The application to transition metal complexes. International Journal of Quantum Chemistry, 1997, 61, 899-918.	1.0	272
113	Calculation of NMR shielding tensors based on density functional theory and a scalar relativistic Pauli-type Hamiltonian. The application to transition metal complexes. , 1997, 61, 899.		7
114	Theoretical Study of13C and17O NMR Shielding Tensors in Transition Metal Carbonyls Based on Density Functional Theory and Gauge-Including Atomic Orbitals. The Journal of Physical Chemistry, 1996, 100, 3359-3367.	2.9	77
115	The Calculation of NMR Parameters by Density-Functional Theory. ACS Symposium Series, 1996, , 328-341.	0.5	13
116	Origin of the Hydridic 1H NMR Chemical Shift in Low-Valent Transition-Metal Hydrides. Organometallics, 1996, 15, 3920-3923.	1.1	99
117	The calculation of77Se chemical shifts using gauge including atomic orbitals and density functional theory. Journal of Chemical Physics, 1996, 104, 8605-8612.	1.2	63
118	The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation. International Journal of Quantum Chemistry, 1996, 60, 753-766.	1.0	153
119	The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation. , 1996, 60, 753.		2
120	The implementation of analytical energy gradients based on a quasi-relativistic density functional method: The application to metal carbonyls. International Journal of Quantum Chemistry, 1995, 56, 477-488.	1.0	42
121	Calculation of NMR Shielding Tensors Using Gauge-Including Atomic Orbitals and Modern Density Functional Theory. The Journal of Physical Chemistry, 1995, 99, 606-611.	2.9	754
122	A Reassessment of the First Metal-Carbonyl Dissociation Energy in M(CO)4 (M = Ni, Pd, Pt), M(CO)5 (M =) Tj ETQq0 0 0 rgBT /Overlock the American Chemical Society, 1995, 117, 486-494.	6.6	435
123	Relativistic Effects on Metal-Ligand Bond Strengths in .pi.-Complexes: Quasi-Relativistic Density Functional Study of M(PH3)2X2 (M = Ni, Pd, Pt; X2 = O2, C2H2, C2H4) and M(CO)4(C2H4) (M = Fe, Ru, Os). Inorganic Chemistry, 1995, 34, 3245-3252.	1.9	95
124	First Bond Dissociation Energy of M(CO)6 (M = Cr, Mo, W) Revisited: The Performance of Density Functional Theory and the Influence of Relativistic Effects. The Journal of Physical Chemistry, 1994, 98, 4838-4841.	2.9	105
125	The Metal Carbon Double Bond in Fischer Carbenes: A Density Functional Study of the Importance of Nonlocal Density Corrections and Relativistic Effects. The Journal of Physical Chemistry, 1994, 98, 11406-11410.	2.9	47
126	Chemical Bonding in Actinyl (V/VI) Dipyriamethyrin Complexes for the Actinide Series from Americium to Californium: A Computational Investigation. Dalton Transactions, 0, , .	1.6	2