Angela K Wilson

List of Publications by Year
in descending order

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170	12,745	66234	24179
papers	citations	42 h-index	110 g-index

176	176	176	8745
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron-nuclear quantum dynamics of diatomic molecules: nonadiabatic signatures in molecular spectra. Molecular Physics, 2022, 120, .	0.8	0
2	Ab Initio Composite Approaches for Heavy Element Energetics: Ionization Potentials for the Actinide Series of Elements. Journal of Physical Chemistry A, 2022, 126, 3027-3042.	1.1	3
3	Adsorption, Structure, and Dynamics of Short- and Long-Chain PFAS Molecules in Kaolinite: Molecular-Level Insights. Environmental Science & Technology, 2022, 56, 8043-8052.	4.6	30
4	Ab initio composite strategies and multireference approaches for lanthanide sulfides and selenides. Journal of Chemical Physics, 2022, 157, .	1.2	6
5	SAMPL7: Hostâ€“guest binding prediction by molecular dynamics and quantum mechanics. Journal of Computer-Aided Molecular Design, 2021, 35, 63-77.	1.3	9
6	Scientific collaboration for a better, more sustainable tomorrow. National Science Review, 2021, 8, nwab035.	4.6	0
7	Multireference calculations on the ground and lowest excited states and dissociation energy of LuF. Journal of Chemical Physics, 2021, 154, 244304.	1.2	4
8	Binding of Per- and Polyfluoro-alkyl Substances to Peroxisome Proliferator-Activated Receptor Gamma. ACS Omega, 2021, 6, 15103-15114.	1.6	19
9	Considering Density Functional Approaches for Actinide Species: The An66 Molecule Set. Journal of Physical Chemistry A, 2021, 125, 7029-7037.	1.1	20
10	Super ccCA (s-ccCA): an approach for accurate transition metal thermochemistry. Molecular Physics, 2021, 119, .	0.8	14
11	Multi-configuration electronâ€“nuclear dynamics: An open-shell approach. Journal of Chemical Physics, 2021, 155, 154103.	1.2	0
12	Ab initio composite methodologies: Their significance for the chemistry community. Annual Reports in Computational Chemistry, 2021, 17, 113-161.	0.9	4
13	Prediction of p K a s of Late Transitionâ€Metal Hydrides via a QM/QM Approach. Journal of Computational Chemistry, 2020, 41, 171-183.	1.5	4
14	Is a High Photoluminescence Quantum Yield Good Enough for OLEDs? Can Luminescence Rigidochromism Be Manifest in the Solid State? an Optoelectronic Device Screening Case Study for Diphosphine/Pyrazolate Copper(I) Complexes. Comments on Inorganic Chemistry, 2020, 40, 1-24.	3.0	6
15	Domainâ€based local pair natural orbital methods within the correlation consistent composite approach. Journal of Computational Chemistry, 2020, 41, 800-813.	1.5	14
16	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadiumâ€“Ligand Bonds. Journal of Physical Chemistry A, 2020, 124, 9757-9770.	1.1	5
17	Computational chemistry considerations in catalysis: Regioselectivity and metal-ligand dissociation. Catalysis Today, 2020, 358, 422-429.	2.2	5
18	Binding of Per- and Polyfluoroalkyl Substances to the Human Pregnane X Receptor. Environmental Science & Technology, 2020, 54, 15986-15995.	4.6	24

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19	Chemical synthesis of human syndecan-4 glycopeptide bearing O-, N-sulfation and multiple aspartic acids for probing impacts of the glycan chain and the core peptide on biological functions. Chemical Science, 2020, 11, 6393-6404.	3.7	18
20	A novel series of cysteine-dependent, allosteric inverse agonists of the nuclear receptor RORÎ³t. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126967.	1.0	11
21	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
22	Correlation consistent basis sets designed for density functional theory: Second-row (Al-Ar). Journal of Chemical Physics, 2019, 151, 064110.	1.2	2
23	Coupled electron and nuclear motion in strong laser fields. Physical Review A, 2019, 100, .	1.0	8
24	Theoretical Studies of Two Key Low-Lying Carbenes of C₅H₂Missing in the Laboratory. Journal of Physical Chemistry A, 2019, 123, 6618-6627.	1.1	18
25	IUPAC Distinguished Women in Chemistry: Contributions to Science and Careers. Pure and Applied Chemistry, 2019, 91, 175-180.	0.9	2
26	Slater and Gaussian basis functions and computation of molecular integrals. , 2019, , 31-61.		0
27	Charge Stabilization in High-Potential Zinc Porphyrin-Fullerene via Axial Ligation of Tetrathiafulvalene. Journal of Physical Chemistry C, 2018, 122, 13636-13647.	1.5	16
28	Impact of intracellular ionic strength on dimer binding in the NF-kB Inducing kinase. Journal of Structural Biology, 2018, 202, 183-190.	1.3	0
29	The role of the CI expansion length in time-dependent studies. Journal of Chemical Physics, 2018, 148, 014107.	1.2	17
30	SAMPL6 hostâ€“guest challenge: binding free energies via a multistep approach. Journal of Computer-Aided Molecular Design, 2018, 32, 1097-1115.	1.3	16
31	Chemoenzymatic synthesis of glycopeptides bearing rare N-glycan sequences with or without bisecting GlcNAc. Chemical Science, 2018, 9, 8194-8206.	3.7	16
32	Adsorption and molecular siting of CO₂, water, and other gases in the superhydrophobic, flexible pores of FMOF-1 from experiment and simulation. Chemical Science, 2017, 8, 3989-4000.	3.7	60
33	Efficacy of Density Functionals and Relativistic Effective Core Potentials for Lanthanide-Containing Species: The Ln54 Molecule Set. Journal of Chemical Theory and Computation, 2017, 13, 2831-2839.	2.3	25
34	Challenges and opportunities for women in science. Nature Reviews Chemistry, 2017, 1, .	13.8	1
35	Relativistic ab Initio Accurate Atomic Minimal Basis Sets: Quantitative LUMOs and Oriented Quasi-Atomic Orbitals for the Elements Liâ€“Xe. Journal of Physical Chemistry A, 2017, 121, 3588-3597.	1.1	18
36	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2017, 13, 4907-4913.	2.3	30

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37	Importance of the ligand basis set in ab initio thermochemical calculations of transition metal species. Chemical Physics Letters, 2017, 685, 496-503.	1.2	2
38	Toward a More Rational Design of the Direct Synthesis of Aniline: A Density Functional Theory Study. ACS Omega, 2017, 2, 3214-3227.	1.6	1
39	Dissociation energy and electronic structure of the low valent lanthanide compound NdF⁺. International Journal of Quantum Chemistry, 2016, 116, 791-794.	1.0	5
40	4-Component relativistic calculations of L₃ionization and excitations for the isoelectronic species UO₂²⁺, OUN⁺and UN₂. Physical Chemistry Chemical Physics, 2016, 18, 21010-21023.	1.3	24
41	DFT and ab initio composite methods: Investigation of oxygen fluoride species. Computational and Theoretical Chemistry, 2016, 1095, 71-82.	1.1	5
42	Partition coefficients for the SAMPL5 challenge using transfer free energies. Journal of Computer-Aided Molecular Design, 2016, 30, 1129-1138.	1.3	19
43	Oxidative Cleavage of the Î²-O-4 Linkage of Lignin by Transition Metals: Catalytic Properties and the Performance of Density Functionals. Journal of Physical Chemistry A, 2016, 120, 737-746.	1.1	25
44	Gauging the Performance of Density Functionals for Lanthanide-Containing Molecules. Journal of Chemical Theory and Computation, 2016, 12, 1259-1266.	2.3	39
45	Ab initio approaches for the determination of heavy element energetics: Ionization energies of trivalent lanthanides (Ln = La-Eu). Journal of Chemical Physics, 2015, 143, 194109.	1.2	15
46	Do composite methods achieve their target accuracy?. Computational and Theoretical Chemistry, 2015, 1072, 58-62.	1.1	17
47	Cleavage of the Î²O4 linkage of lignin using group 8 pincer complexes: A DFT study. Journal of Molecular Catalysis A, 2015, 399, 33-41.	4.8	19
48	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	26
49	Pseudopotential-Based Correlation Consistent Composite Approach (rp-ccCA) for First- and Second-Row Transition Metal Thermochemistry. Journal of Physical Chemistry A, 2015, 119, 6867-6874.	1.1	24
50	Correlation consistent basis sets for the atoms Inâ€“Xe. Journal of Chemical Physics, 2015, 142, 084102.	1.2	4
51	Multireference Character for 4d Transition Metal-Containing Molecules. Journal of Chemical Theory and Computation, 2015, 11, 5865-5872.	2.3	86
52	A Computational Study on the Ground and Excited States of Nickel Silicide. Journal of Physical Chemistry A, 2015, 119, 9630-9635.	1.1	5
53	Behavior of the Sapporo-nZP-2012 basis set family. Chemical Physics Letters, 2015, 637, 120-126.	1.2	8
54	Ground and Excited Electronic State Analysis of PrF²⁺ and PmF²⁺. Journal of Physical Chemistry A, 2015, 119, 1683-1688.	1.1	7

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55	Bonding and Phosphorescence Trends in 1-D, 2-D, and 3-D Oligomers and Extended Excimers of Group 12 Metals: Validation of Cooperativity in Both Metallophilic and Excimeric Bonding. Journal of Physical Chemistry C, 2015, 119, 2015-2028.	1.5	3
56	The Importance of Orbital Analysis. Progress in Theoretical Chemistry and Physics, 2015, , 3-28.	0.2	0
57	Low valency in lanthanides: A theoretical study of NdF and LuF. Journal of Chemical Physics, 2014, 140, 224314.	1.2	17
58	Selectivity in ROS-Induced Peptide Backbone Bond Cleavage. Journal of Physical Chemistry A, 2014, 118, 11399-11404.	1.1	18
59	Molecular Dynamics Studies of the Proteinâ€“Protein Interactions in Inhibitor of Î²B Kinase-Î². Journal of Chemical Information and Modeling, 2014, 54, 562-572.	2.5	13
60	Solv-ccCA: Implicit Solvation and the Correlation Consistent Composite Approach for the Determination of pK_a. Journal of Chemical Theory and Computation, 2014, 10, 1500-1510.	2.3	21
61	Highâ€Potential Perfluorinated Phthalocyanineâ€“Fullerene Dyads for Generation of Highâ€Energy Chargeâ€Separated States: Formation and Photoinduced Electronâ€Transfer Studies. ChemPhysChem, 2014, 15, 2462-2472.	1.0	41
62	Electron Transfer Studies of High Potential Zinc Porphyrinâ€“Fullerene Supramolecular Dyads. Journal of Physical Chemistry C, 2014, 118, 3994-4006.	1.5	103
63	MR-ccCA: A route for accurate ground and excited state potential energy curves and spectroscopic properties for third-row diatomic molecules. Computational and Theoretical Chemistry, 2014, 1040-1041, 72-83.	1.1	9
64	Performance of Density Functional Theory for Second Row (4d) Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2013, 9, 3939-3946.	2.3	74
65	A Neoteric Neodymium Model: Ground and Excited Electronic State Analysis of NdF^{2+}. Journal of Physical Chemistry A, 2013, 117, 10881-10888.	1.1	10
66	Complete basis set limits of local second-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2013, 111, 1178-1189.	0.8	0
67	Bonding properties of seleniumâ€“carbon complexes: Computational modeling of H3CSeH, H2CSe, HOCSeH, H2CSeO, SeC and HCSeOH. Computational and Theoretical Chemistry, 2013, 1017, 41-47.	1.1	1
68	Periodic Trends in 3d Metal Mediated CO2 Activation. ACS Symposium Series, 2013, , 67-88.	0.5	3
69	Câ€“O Bond Cleavage of Dimethyl Ether by Transition Metal Ions: A Systematic Study on Catalytic Properties of Metals and Performance of DFT Functionals. Journal of Physical Chemistry A, 2013, 117, 5140-5148.	1.1	26
70	Spectroscopic properties of Arxâ€“Zn and Arxâ€“Ag+(x= 1,2) van der Waals complexes. Journal of Chemical Physics, 2013, 138, 104116.	1.2	1
71	Cooperative Carbon Capture Capabilities in Multivariate MOFs Decorated with Amino Acid Side Chains: A Computational Study. Journal of Physical Chemistry C, 2013, 117, 14717-14722.	1.5	13
72	Explicitly Correlated Methods within the ccCA Methodology. Journal of Chemical Theory and Computation, 2013, 9, 1402-1407.	2.3	26

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73	Incorporating a completely renormalized coupled cluster approach into a composite method for thermodynamic properties and reaction paths. Journal of Chemical Physics, 2012, 136, 144109.	1.2	26
74	Interaction Energies of CO2Â·Amine Complexes: Effects of Amine Substituents. Journal of Physical Chemistry A, 2012, 116, 10403-10411.	1.1	9
75	Examining the heavy p-block with a pseudopotential-based composite method: Atomic and molecular applications of rp-ccCA. Journal of Chemical Physics, 2012, 137, 214111.	1.2	14
76	Carbon Dioxide Migration Pathways in Proteins. Journal of Physical Chemistry Letters, 2012, 3, 830-833.	2.1	9
77	Nature of Proteinâ€“CO₂ Interactions as Elucidated via Molecular Dynamics. Journal of Physical Chemistry B, 2012, 116, 11578-11593.	1.2	7
78	Comparative Study of Single and Double Hybrid Density Functionals for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2012, 8, 4102-4111.	2.3	69
79	Multireference Character for 3d Transition-Metal-Containing Molecules. Journal of Chemical Theory and Computation, 2012, 8, 460-468.	2.3	237
80	Empirical Correction of Nondynamical Correlation Energy for Density Functionals. Journal of Physical Chemistry A, 2012, 116, 9969-9978.	1.1	16
81	Enthalpies of formation for organosulfur compounds: Atomization energy and hypohomodesmotic reaction schemes via ab initio composite methods. Computational and Theoretical Chemistry, 2012, 991, 1-12.	1.1	10
82	Proton affinities of deoxyribonucleosides via the ONIOMâ€ccCA methodology. Journal of Computational Chemistry, 2012, 33, 2590-2601.	1.5	6
83	Ab Initio Composite Approaches. Annual Reports in Computational Chemistry, 2012, 8, 29-51.	0.9	3
84	CO₂ Reduction on Transition Metal (Fe, Co, Ni, and Cu) Surfaces: In Comparison with Homogeneous Catalysis. Journal of Physical Chemistry C, 2012, 116, 5681-5688.	1.5	247
85	Comment on the paper â€œExtensive Theoretical Studies of a New Energetic Material: Tetrazino-Tetrazine-Tetraoxide (TTTO)â€•by Xinli Song, Jicun Li, Hua Hou, and Baoshan Wang. Journal of Computational Chemistry, 2012, 33, 1967-1968.	1.5	3
86	Prediction of hydrocarbon enthalpies of formation by various thermochemical schemes. Journal of Computational Chemistry, 2012, 33, 2032-2042.	1.5	14
87	Vibrational frequency scale factors for density functional theory and the polarization consistent basis sets. Journal of Computational Chemistry, 2012, 33, 2380-2387.	1.5	186
88	Proteinâ€based carbon capture: progress and potential. , 2012, 2, 223-238.		12
89	Toward Accurate Theoretical Thermochemistry of First Row Transition Metal Complexes. Journal of Physical Chemistry A, 2012, 116, 870-885.	1.1	138
90	The importance of secondary structure in determining CO2-protein binding patterns. Journal of Molecular Modeling, 2012, 18, 2527-2541.	0.8	4

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91	Theoretical prediction of FKrOH. Chemical Physics Letters, 2012, 537, 6-10.	1.2	4
92	Modeling the Photophysics of Zn and Cd Monomers, Metallophilic Dimers, and Covalent Excimers. Journal of Physical Chemistry A, 2011, 115, 374-382.	1.1	9
93	Reaction Mechanism of the Reverse Waterâ€“Gas Shift Reaction Using First-Row Middle Transition Metal Catalysts Lâ€²M (M = Fe, Mn, Co): A Computational Study. Inorganic Chemistry, 2011, 50, 8782-8789.	1.9	27
94	Gaussian basis sets for use in correlated molecular calculations. VII. Valence, core-valence, and scalar relativistic basis sets for Li, Be, Na, and Mg. Theoretical Chemistry Accounts, 2011, 128, 69-82.	0.5	536
95	Oxidative Addition of the C_{Î±}ï£¿C_{Î²} Bond in Î²â€Oâ€4 Linkage of Lignin to Transition Metals Using a Relativistic Pseudopotentialâ€Based ccCAâ€ONIOM Method. ChemPhysChem, 2011, 12, 3320-3330.	1.0	26
96	Harmonic vibrational frequencies: Scale factors for pure, hybrid, hybrid meta, and doubleâ€hybrid functionals in conjunction with correlation consistent basis sets. Journal of Computational Chemistry, 2011, 32, 2339-2347.	1.5	61
97	The correlation Consistent composite Approach: The spin contamination effect on an MP2-based composite methodology. Chemical Physics Letters, 2011, 504, 88-94.	1.2	21
98	Highly energetic nitrogen species: Reliable energetics via the correlation consistent Composite Approach (ccCA). Journal of Hazardous Materials, 2011, 186, 583-589.	6.5	58
99	Multireference composite approaches for the accurate study of ground and excited electronic states: C2, N2, and O2. Journal of Chemical Physics, 2011, 134, 034101.	1.2	45
100	A pseudopotential-based composite method: The relativistic pseudopotential correlation consistent composite approach for molecules containing 4d transition metals (Yâ€“Cd). Journal of Chemical Physics, 2011, 135, 214103.	1.2	39
101	Accurate predictions of the energetics of silicon compounds using the multireference correlation consistent composite approach. Journal of Chemical Physics, 2011, 135, 094103.	1.2	22
102	A QM/QM Multilayer Composite Methodology: The ONIOM Correlation Consistent Composite Approach (ONIOM-ccCA). Journal of Physical Chemistry A, 2010, 114, 9394-9397.	1.1	17
103	Toward Greener Carbon Capture Technologies: A Pharmacophore-Based Approach to Predict CO₂ Binding Sites in Proteins. Energy & Fuels, 2010, 24, 1464-1470.	2.5	5
104	Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. Physical Review B, 2010, 81, .	1.1	31
105	First-principle study of structure and stability of nickel carbides. Journal of Physics Condensed Matter, 2010, 22, 445503.	0.7	34
106	Multireference Correlation Consistent Composite Approach [MR-ccCA]: Toward Accurate Prediction of the Energetics of Excited and Transition State Chemistry^{â€}. Journal of Physical Chemistry A, 2010, 114, 8806-8816.	1.1	36
107	Theoretical Studies on the Catalysis of the Reverse Waterâ^'Gas Shift Reaction Using First-Row Transition Metal Î²-Diketiminato Complexes. Journal of Physical Chemistry A, 2010, 114, 6207-6216.	1.1	23
108	The resolution of the identity approximation applied to the correlation consistent composite approach. Journal of Chemical Physics, 2009, 131, 044130.	1.2	21

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109	Computation of potential energy surfaces with the multireference correlation consistent composite approach. Journal of Chemical Physics, 2009, 130, 234104.	1.2	32
110	A CCSD(T) and ccCA study of mixed silicon hydrides and halides: Structures and thermochemistry. Chemical Physics, 2009, 359, 1-13.	0.9	18
111	Basis set requirements for interactions in ionic systems: LiCl. Chemical Physics Letters, 2009, 468, 286-289.	1.2	4
112	Accurate thermochemistry for transition metal complexes from first-principles calculations. Journal of Chemical Physics, 2009, 131, 024106.	1.2	95
113	CO₂-Formatics: How Do Proteins Bind Carbon Dioxide?. Journal of Chemical Information and Modeling, 2009, 49, 2111-2115.	2.5	44
114	Structures and Thermochemistry of the Alkali Metal Monoxide Anions, Monoxide Radicals, and Hydroxides. Journal of Physical Chemistry A, 2009, 113, 9501-9510.	1.1	17
115	Enthalpy of Formation of the Cyclohexadienyl Radical and the Câ^'H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-Evaluation. Journal of Physical Chemistry A, 2009, 113, 6955-6963.	1.1	47
116	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	0.8	96
117	Performance of Density Functional Theory for 3d Transition Metal-Containing Complexes: Utilization of the Correlation Consistent Basis Sets. Journal of Physical Chemistry A, 2009, 113, 8607-8614.	1.1	84
118	The Correlation Consistent Composite Approach (ccCA): Efficient and Pan-Periodic Kinetics and Thermodynamics. Progress in Theoretical Chemistry and Physics, 2009, , 197-224.	0.2	13
119	Core-valence correlation consistent basis sets for second-row atoms (Alâ€“Ar) revisited. Theoretical Chemistry Accounts, 2008, 120, 119-131.	0.5	26
120	Theoretical investigation of the germanium arsenides. Chemical Physics, 2008, 353, 209-220.	0.9	2
121	Importance of the quality of metal and ligand basis sets in transition metal species. Journal of Chemical Physics, 2008, 129, 054108.	1.2	8
122	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	1.2	367
123	Application of the Correlation Consistent Composite Approach (ccCA) to Third-Row (Gaâ^'Kr) Molecules. Journal of Chemical Theory and Computation, 2008, 4, 328-334.	2.3	46
124	Hartree-Fock complete basis set limit properties for transition metal diatomics. Journal of Chemical Physics, 2008, 128, 044101.	1.2	34
125	Performance of the correlation-consistent composite approach for sulfur species. Journal of Sulfur Chemistry, 2008, 29, 353-365.	1.0	19
126	Performance of the correlation consistent composite approach for transition states: A comparison to G3B theory. Journal of Chemical Physics, 2007, 127, 154117.	1.2	34

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127	Behavior of density functionals with respect to basis set. VI. Truncation of the correlation consistent basis sets. Journal of Chemical Physics, 2007, 127, 124110.	1.2	19
128	Structure and Stability of the Organo-Noble Gas Molecules XNgCCX and XNgCCNgX (Ng = Kr, Ar; X = F,) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	15
129	Photophysics and Bonding in Neutral Gold(I) Organometallic Complexes with an Extended Aurophilic Supramolecular Structure. Organometallics, 2007, 26, 2550-2560.	1.1	34
130	Systematically Convergent Correlation Consistent Basis Sets for Molecular Coreâ^'Valence Correlation Effects:â€‰ The Third-Row Atoms Gallium through Krypton. Journal of Physical Chemistry A, 2007, 111, 11383-11393.	1.1	138
131	Quantitative Computational Thermochemistry of Transition Metal Species. Journal of Physical Chemistry A, 2007, 111, 11269-11277.	1.1	153
132	Computationals-Block Thermochemistry with the Correlation Consistent Composite Approach. Journal of Physical Chemistry A, 2007, 111, 10776-10780.	1.1	46
133	Photophysics of Bis(thiocyanato)gold(I) Complexes:â€‰ Intriguing Structureâ^'Luminescence Relationships. Journal of Physical Chemistry C, 2007, 111, 10689-10699.	1.5	47
134	The behaviour of density functionals with respect to basis set. V. Recontraction of correlation consistent basis sets. Molecular Physics, 2007, 105, 2899-2917.	0.8	21
135	A computational study of dihalogen-Î¼-dichalcogenides: XAAX (X=F, Cl, Br; A=S, Se). Computational and Theoretical Chemistry, 2007, 814, 1-10.	1.5	32
136	Truncation of the correlation consistent basis sets: Application to extended systems. International Journal of Quantum Chemistry, 2007, 107, 3077-3088.	1.0	1
137	Behavior of Density Functionals with Respect to Basis Set. 3. Basis Set Superposition Errorâ€. Journal of Physical Chemistry A, 2006, 110, 779-784.	1.1	30
138	Accurate Enthalpies of Formation of Alkali and Alkaline Earth Metal Oxides and Hydroxides:Â Assessment of the Correlation Consistent Composite Approach (ccCA). Journal of Physical Chemistry A, 2006, 110, 9767-9770.	1.1	47
139	The correlation consistent composite approach (ccCA): An alternative to the Gaussian-n methods. Journal of Chemical Physics, 2006, 124, 114104.	1.2	269
140	Computation of gas-phase enthalpies of formation with chemical accuracy: The curious case of 3-nitroaniline. Computational and Theoretical Chemistry, 2006, 775, 77-80.	1.5	22
141	The correlation-consistent composite approach: Application to the G3/99 test set. Journal of Chemical Physics, 2006, 125, 104111.	1.2	134
142	Calculation of the enthalpies of formation for transition metal complexes. Chemical Physics Letters, 2005, 401, 58-61.	1.2	48
143	The existence of FKrCF3, FKrSiF3, and FKrGeF3: A theoretical study. Chemical Physics Letters, 2005, 411, 91-97.	1.2	22
144	Behaviour of density functionals with respect to basis set: II. Polarization consistent basis sets. Molecular Physics, 2005, 103, 345-358.	0.8	32

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145	Truncation of the correlation consistent basis sets: Extension to third-row (Gaâ€“Kr) molecules. Journal of Chemical Physics, 2005, 122, 134106.	1.2	10
146	Relativistic effects determined using the Douglasâ€“Kroll contracted basis sets and correlation consistent basis sets with small-core relativistic pseudopotentials. Journal of Chemical Physics, 2005, 122, 174310.	1.2	15
147	Density Functional Theory and the Correlation Consistent Basis Sets:â€‰ The Tight d Effect on HSO and HOS. Journal of Physical Chemistry A, 2005, 109, 7187-7196.	1.1	43
148	Structures and Thermochemistry of Calcium-Containing Molecules. Journal of Physical Chemistry A, 2005, 109, 9156-9168.	1.1	17
149	Electronic Structure of Mercury Oligomers and Exciplexes:Â Models for Long-Range/Multicenter Bonding in Phosphorescent Transition-Metal Compounds. Journal of Physical Chemistry A, 2005, 109, 690-702.	1.1	21
150	Beyond a T-Shape. Journal of the American Chemical Society, 2005, 127, 12488-12489.	6.6	77
151	Truncation of the correlation consistent basis sets: An effective approach to the reduction of computational cost?. Journal of Chemical Physics, 2004, 121, 5629-5634.	1.2	16
152	Accurate energetics of small molecules containing third-row atoms Gaâ€“Kr: A comparison of advanced ab initio and density functional theory. Journal of Chemical Physics, 2004, 121, 60.	1.2	18
153	The behavior of density functionals with respect to basis set. I. The correlation consistent basis sets. Journal of Chemical Physics, 2004, 121, 7632.	1.2	98
154	An ab initio study of the noble gas compound HKrCl. Chemical Physics Letters, 2004, 393, 448-452.	1.2	19
155	SO3 revisited: Impact of tight d augmented correlation consistent basis sets on atomization energy and structure. Chemical Physics Letters, 2004, 394, 105-109.	1.2	28
156	The HSOâ^'SOH Isomers Revisited:Â The Effect of Tight d Functionsâ€. Journal of Physical Chemistry A, 2004, 108, 3129-3133.	1.1	104
157	Harmonic Vibrational Frequencies:â€‰ Scaling Factors for HF, B3LYP, and MP2 Methods in Combination with Correlation Consistent Basis Sets. Journal of Physical Chemistry A, 2004, 108, 9213-9217.	1.1	405
158	Effects of Basis Set Choice upon the Atomization Energy of the Second-Row Compounds SO2, CCl, and ClO2 for B3LYP and B3PW91. Journal of Physical Chemistry A, 2003, 107, 6720-6724.	1.1	50
159	SO2 revisited: Impact of tight d augmented correlation consistent basis sets on structure and energetics. Journal of Chemical Physics, 2003, 119, 11712-11714.	1.2	83
160	Gaussian basis sets for use in correlated molecular calculations. X. The atoms aluminum through argon revisited. Journal of Chemical Physics, 2001, 114, 9244-9253.	1.2	1,463
161	Gaussian basis sets for use in correlated molecular calculations. IX. The atoms gallium through krypton. Journal of Chemical Physics, 1999, 110, 7667-7676.	1.2	1,309
162	Benchmark calculations with correlated molecular wavefunctions. XIII. Potential energy curves for He2, Ne2 and Ar2 using correlation consistent basis sets through augmented sextuple zeta. Molecular Physics, 1999, 96, 529-547.	0.8	254

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163	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
164	The Effect of Basis Set Superposition Error (BSSE) on the Convergence of Molecular Properties Calculated with the Correlation Consistent Basis Sets. Advances in Quantum Chemistry, 1998, 31, 105-135.	0.4	80
165	A semiclassical study of tunneling effects in aziridine. Journal of Chemical Physics, 1998, 109, 9258-9262.	1.2	8
166	Benchmark calculations with correlated molecular wave functions. X. Comparison with â€œexactâ€•MP2 calculations on Ne, HF, H2O, and N2. Journal of Chemical Physics, 1997, 106, 8718-8726.	1.2	166
167	MÃ¸ller-Plesset correlation energies in a localized orbital basis using a Laplace transform technique. Theoretica Chimica Acta, 1997, 95, 49-62.	0.9	25
168	Benchmark calculations with correlated molecular wave functions. Theoretical Chemistry Accounts, 1997, 97, 251-259.	0.5	129
169	MÃ¸llerâ€“Plesset correlation energies in a localized orbital basis using a Laplace transform technique. Theoretica Chimica Acta, 1997, 95, 49.	0.9	33
170	Gaussian basis sets for use in correlated molecular calculations. VI. Sextuple zeta correlation consistent basis sets for boron through neon. Computational and Theoretical Chemistry, 1996, 388, 339-349.	1.5	1,013