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	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
2	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
3	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
4	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
5	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
6	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
7	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	1.2	367
8	The correlation consistent composite approach (ccCA): An alternative to the Gaussian-n methods. Journal of Chemical Physics, 2006, 124, 114104.	1.2	269
9	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
10	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
11	Multireference Character for 3d Transition-Metal-Containing Molecules. Journal of Chemical Theory and Computation, 2012, 8, 460-468.	2.3	237
12	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
13	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
14	Quantitative Computational Thermochemistry of Transition Metal Species. Journal of Physical Chemistry A, 2007, 111, 11269-11277.	1.1	153
15	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
16	Toward Accurate Theoretical Thermochemistry of First Row Transition Metal Complexes. Journal of Physical Chemistry A, 2012, 116, 870-885.	1.1	138
17	The correlation-consistent composite approach: Application to the G3/99 test set. Journal of Chemical Physics, 2006, 125, 104111.	1.2	134
18	Benchmark calculations with correlated molecular wave functions. Theoretical Chemistry Accounts, 1997, 97, 251-259.	0.5	129

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19	The HSOâ^'SOH Isomers Revisited:Â The Effect of Tight d Functionsâ€. Journal of Physical Chemistry A, 2004, 108, 3129-3133.	1.1	104
20	Electron Transfer Studies of High Potential Zinc Porphyrinâ€“Fullerene Supramolecular Dyads. Journal of Physical Chemistry C, 2014, 118, 3994-4006.	1.5	103
21	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
22	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	0.8	96
23	Accurate thermochemistry for transition metal complexes from first-principles calculations. Journal of Chemical Physics, 2009, 131, 024106.	1.2	95
24	Multireference Character for 4d Transition Metal-Containing Molecules. Journal of Chemical Theory and Computation, 2015, 11, 5865-5872.	2.3	86
25	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
26	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
27	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
28	Beyond a T-Shape. Journal of the American Chemical Society, 2005, 127, 12488-12489.	6.6	77
29	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
30	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
31	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
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	Highly energetic nitrogen species: Reliable energetics via the correlation consistent Composite Approach (ccCA). Journal of Hazardous Materials, 2011, 186, 583-589.	6.5	58
34	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
35	Calculation of the enthalpies of formation for transition metal complexes. Chemical Physics Letters, 2005, 401, 58-61.	1.2	48
36	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

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37	Photophysics of Bis(thiocyanato)gold(I) Complexes:â€‰ Intriguing Structureâ^'Luminescence Relationships. Journal of Physical Chemistry C, 2007, 111, 10689-10699.	1.5	47
38	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
39	Computationals-Block Thermochemistry with the Correlation Consistent Composite Approach. Journal of Physical Chemistry A, 2007, 111, 10776-10780.	1.1	46
40	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
41	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
42	CO₂-Formatics: How Do Proteins Bind Carbon Dioxide?. Journal of Chemical Information and Modeling, 2009, 49, 2111-2115.	2.5	44
43	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
44	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
45	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
46	Gauging the Performance of Density Functionals for Lanthanide-Containing Molecules. Journal of Chemical Theory and Computation, 2016, 12, 1259-1266.	2.3	39
47	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
48	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
49	Photophysics and Bonding in Neutral Gold(I) Organometallic Complexes with an Extended Aurophilic Supramolecular Structure. Organometallics, 2007, 26, 2550-2560.	1.1	34
50	Hartree-Fock complete basis set limit properties for transition metal diatomics. Journal of Chemical Physics, 2008, 128, 044101.	1.2	34
51	First-principle study of structure and stability of nickel carbides. Journal of Physics Condensed Matter, 2010, 22, 445503.	0.7	34
52	MÃ¸llerâ€“Plesset correlation energies in a localized orbital basis using a Laplace transform technique. Theoretica Chimica Acta, 1997, 95, 49.	0.9	33
53	Behaviour of density functionals with respect to basis set: II. Polarization consistent basis sets. Molecular Physics, 2005, 103, 345-358.	0.8	32
54	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

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55	Computation of potential energy surfaces with the multireference correlation consistent composite approach. Journal of Chemical Physics, 2009, 130, 234104.	1.2	32
56	Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. Physical Review B, 2010, 81, .	1.1	31
57	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
58	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
59	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
60	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
61	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
62	Core-valence correlation consistent basis sets for second-row atoms (Alâ€“Ar) revisited. Theoretical Chemistry Accounts, 2008, 120, 119-131.	0.5	26
63	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
64	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
65	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
66	Explicitly Correlated Methods within the ccCA Methodology. Journal of Chemical Theory and Computation, 2013, 9, 1402-1407.	2.3	26
67	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	26
68	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
69	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
70	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
71	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
72	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

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73	Binding of Per- and Polyfluoroalkyl Substances to the Human Pregnane X Receptor. Environmental Science & Technology, 2020, 54, 15986-15995.	4.6	24
74	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
75	The existence of FKrCF3, FKrSiF3, and FKrGeF3: A theoretical study. Chemical Physics Letters, 2005, 411, 91-97.	1.2	22
76	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
77	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
78	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
79	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
80	The resolution of the identity approximation applied to the correlation consistent composite approach. Journal of Chemical Physics, 2009, 131, 044130.	1.2	21
81	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
82	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
83	Considering Density Functional Approaches for Actinide Species: The An66 Molecule Set. Journal of Physical Chemistry A, 2021, 125, 7029-7037.	1.1	20
84	An ab initio study of the noble gas compound HKrCl. Chemical Physics Letters, 2004, 393, 448-452.	1.2	19
85	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
86	Performance of the correlation-consistent composite approach for sulfur species. Journal of Sulfur Chemistry, 2008, 29, 353-365.	1.0	19
87	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
88	Partition coefficients for the SAMPL5 challenge using transfer free energies. Journal of Computer-Aided Molecular Design, 2016, 30, 1129-1138.	1.3	19
89	Binding of Per- and Polyfluoro-alkyl Substances to Peroxisome Proliferator-Activated Receptor Gamma. ACS Omega, 2021, 6, 15103-15114.	1.6	19
90	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

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91	A CCSD(T) and ccCA study of mixed silicon hydrides and halides: Structures and thermochemistry. Chemical Physics, 2009, 359, 1-13.	0.9	18
92	Selectivity in ROS-Induced Peptide Backbone Bond Cleavage. Journal of Physical Chemistry A, 2014, 118, 11399-11404.	1.1	18
93	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
94	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
95	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
96	Structures and Thermochemistry of Calcium-Containing Molecules. Journal of Physical Chemistry A, 2005, 109, 9156-9168.	1.1	17
97	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
98	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
99	Low valency in lanthanides: A theoretical study of NdF and LuF. Journal of Chemical Physics, 2014, 140, 224314.	1.2	17
100	Do composite methods achieve their target accuracy?. Computational and Theoretical Chemistry, 2015, 1072, 58-62.	1.1	17
101	The role of the CI expansion length in time-dependent studies. Journal of Chemical Physics, 2018, 148, 014107.	1.2	17
102	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
103	Empirical Correction of Nondynamical Correlation Energy for Density Functionals. Journal of Physical Chemistry A, 2012, 116, 9969-9978.	1.1	16
104	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
105	SAMPL6 hostâ€“guest challenge: binding free energies via a multistep approach. Journal of Computer-Aided Molecular Design, 2018, 32, 1097-1115.	1.3	16
106	Chemoenzymatic synthesis of glycopeptides bearing rare N-glycan sequences with or without bisecting GlcNAc. Chemical Science, 2018, 9, 8194-8206.	3.7	16
107	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
108	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

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109	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
110	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
111	Prediction of hydrocarbon enthalpies of formation by various thermochemical schemes. Journal of Computational Chemistry, 2012, 33, 2032-2042.	1.5	14
112	Domainâ€based local pair natural orbital methods within the correlation consistent composite approach. Journal of Computational Chemistry, 2020, 41, 800-813.	1.5	14
113	Super ccCA (s-ccCA): an approach for accurate transition metal thermochemistry. Molecular Physics, 2021, 119, .	0.8	14
114	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
115	Molecular Dynamics Studies of the Proteinâ€"Protein Interactions in Inhibitor of ÎºB Kinase-Î². Journal of Chemical Information and Modeling, 2014, 54, 562-572.	2.5	13
116	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
117	Proteinâ€based carbon capture: progress and potential. , 2012, 2, 223-238.		12
118	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
119	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
120	Truncation of the correlation consistent basis sets: Extension to third-row (Gaâ€"Kr) molecules. Journal of Chemical Physics, 2005, 122, 134106.	1.2	10
121	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
122	A Neoteric Neodymium Model: Ground and Excited Electronic State Analysis of NdF²⁺. Journal of Physical Chemistry A, 2013, 117, 10881-10888.	1.1	10
123	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
124	Interaction Energies of CO2Â·Amine Complexes: Effects of Amine Substituents. Journal of Physical Chemistry A, 2012, 116, 10403-10411.	1.1	9
125	Carbon Dioxide Migration Pathways in Proteins. Journal of Physical Chemistry Letters, 2012, 3, 830-833.	2.1	9
126	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

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127	SAMPL7: Hostâ€“guest binding prediction by molecular dynamics and quantum mechanics. Journal of Computer-Aided Molecular Design, 2021, 35, 63-77.	1.3	9
128	A semiclassical study of tunneling effects in aziridine. Journal of Chemical Physics, 1998, 109, 9258-9262.	1.2	8
129	Importance of the quality of metal and ligand basis sets in transition metal species. Journal of Chemical Physics, 2008, 129, 054108.	1.2	8
130	Behavior of the Sapporo-nZP-2012 basis set family. Chemical Physics Letters, 2015, 637, 120-126.	1.2	8
131	Coupled electron and nuclear motion in strong laser fields. Physical Review A, 2019, 100, .	1.0	8
132	Nature of Proteinâ€“CO₂ Interactions as Elucidated via Molecular Dynamics. Journal of Physical Chemistry B, 2012, 116, 11578-11593.	1.2	7
133	Ground and Excited Electronic State Analysis of PrF²⁺ and PmF²⁺. Journal of Physical Chemistry A, 2015, 119, 1683-1688.	1.1	7
134	Proton affinities of deoxyribonucleosides via the ONIOMâ€ccCA methodology. Journal of Computational Chemistry, 2012, 33, 2590-2601.	1.5	6
135	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
136	Ab initio composite strategies and multireference approaches for lanthanide sulfides and selenides. Journal of Chemical Physics, 2022, 157, .	1.2	6
137	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
138	A Computational Study on the Ground and Excited States of Nickel Silicide. Journal of Physical Chemistry A, 2015, 119, 9630-9635.	1.1	5
139	Dissociation energy and electronic structure of the low valent lanthanide compound NdF⁺. International Journal of Quantum Chemistry, 2016, 116, 791-794.	1.0	5
140	DFT and ab initio composite methods: Investigation of oxygen fluoride species. Computational and Theoretical Chemistry, 2016, 1095, 71-82.	1.1	5
141	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
142	Computational chemistry considerations in catalysis: Regioselectivity and metal-ligand dissociation. Catalysis Today, 2020, 358, 422-429.	2.2	5
143	Basis set requirements for interactions in ionic systems: LiCl. Chemical Physics Letters, 2009, 468, 286-289.	1.2	4
144	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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145	Theoretical prediction of FKrOH. Chemical Physics Letters, 2012, 537, 6-10.	1.2	4
146	Correlation consistent basis sets for the atoms Inâ€“Xe. Journal of Chemical Physics, 2015, 142, 084102.	1.2	4
147	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
148	Multireference calculations on the ground and lowest excited states and dissociation energy of LuF. Journal of Chemical Physics, 2021, 154, 244304.	1.2	4
149	Ab initio composite methodologies: Their significance for the chemistry community. Annual Reports in Computational Chemistry, 2021, 17, 113-161.	0.9	4
150	Ab Initio Composite Approaches. Annual Reports in Computational Chemistry, 2012, 8, 29-51.	0.9	3
151	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
152	Periodic Trends in 3d Metal Mediated CO2 Activation. ACS Symposium Series, 2013, , 67-88.	0.5	3
153	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
154	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
155	Theoretical investigation of the germanium arsenides. Chemical Physics, 2008, 353, 209-220.	0.9	2
156	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
157	Correlation consistent basis sets designed for density functional theory: Second-row (Al-Ar). Journal of Chemical Physics, 2019, 151, 064110.	1.2	2
158	IUPAC Distinguished Women in Chemistry: Contributions to Science and Careers. Pure and Applied Chemistry, 2019, 91, 175-180.	0.9	2
159	Truncation of the correlation consistent basis sets: Application to extended systems. International Journal of Quantum Chemistry, 2007, 107, 3077-3088.	1.0	1
160	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
161	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
162	Challenges and opportunities for women in science. Nature Reviews Chemistry, 2017, 1, .	13.8	1

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163	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
164	Complete basis set limits of local second-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2013, 111, 1178-1189.	0.8	0
165	Impact of intracellular ionic strength on dimer binding in the NF-κB Inducing kinase. Journal of Structural Biology, 2018, 202, 183-190.	1.3	0
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