Kirk A Peterson

List of Publications by Year
in descending order

274	31,231	10986 71	4432 172
papers	citations	h-index	g-index

281	281	281	12724
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interaction of Th with H^{0/â€“/+}: Combined Experimental and Theoretical Thermodynamic Properties. Journal of Physical Chemistry A, 2022, 126, 198-210.	2.5	9
2	ThAu2â¯, ThAu2Oâ¯, and ThAuOHâ¯ anions: Photoelectron spectroscopic and theoretical characterization. Journal of Chemical Physics, 2022, 156, 054305.	3.0	2
3	A high level theory investigation on the lowest-lying ionization potentials of glycine (NH₂CH₂COOH). Physical Chemistry Chemical Physics, 2022, 24, 17751-17758.	2.8	1
4	Improving the theoretical description of Ln(<scp>iii</scp>)/An(<scp>iii</scp>) separation with phosphinic acid ligands: a benchmarking study of structure and selectivity. Physical Chemistry Chemical Physics, 2021, 23, 19558-19570.	2.8	6
5	Benchmarking Antioxidant-Related Properties for Gallic Acid through the Use of DFT, MP2, CCSD, and CCSD(T) Approaches. Journal of Physical Chemistry A, 2021, 125, 198-208.	2.5	49
6	Bond Dissociation Energies in Heavy Element Chalcogen and Halogen Small Molecules. Journal of Physical Chemistry A, 2021, 125, 1892-1902.	2.5	10
7	The electron affinity of the uranium atom. Journal of Chemical Physics, 2021, 154, 224307.	3.0	13
8	Coupled Cluster Studies of Platinumâ€“Actinide Interactions. Thermochemistry of PtAnOⁿ⁺ (n = 0â€“2 and An = U, Np, Pu). Journal of Physical Chemistry A, 2021, 125, 5335-5345.	2.5	6
9	Guided Ion Beam Studies of the Thorium Monocarbonyl Cation Bond Dissociation Energy and Theoretical Unveiling of Different Isomers of [Th,O,C]⁺ and Their Rearrangement Mechanism. Inorganic Chemistry, 2021, 60, 10426-10438.	4.0	5
10	Ionization potentials for the H2CO trimer. Journal of Chemical Physics, 2021, 155, 084304.	3.0	4
11	Nonadiabatic Dynamics at the Gasâ€“Molten Metal Interface: State-to-State Resolved Scattering of NO from Hot Gallium (600â€“1000 K). Journal of Physical Chemistry C, 2021, 125, 341-353.	3.1	3
12	Polarizabilities of neutral atoms and atomic ions with a noble gas electron configuration. Journal of Chemical Physics, 2020, 153, 174304.	3.0	6
13	Calculated Ionization Potentials of MO₃ and MO₂ for M = U, Mo, W, and Nd. Journal of Physical Chemistry A, 2020, 124, 6913-6919.	2.5	9
14	A Computational Assessment of Actinide Dioxide Cations AnO₂²⁺ for An = U to Lr: The Limited Stability Range of the Hexavalent Actinyl Moiety, [Oâ•Anâ•O]²⁺. Inorganic Chemistry, 2020, 59, 4554-4566.	4.0	17
15	Probing the ionization potentials of the formaldehyde dimer. Journal of Chemical Physics, 2020, 152, 194305.	3.0	6
16	Coupled Cluster Study of the Interactions of AnO₂, AnO₂⁺, and AnO₂²⁺ (An = U, Np) with N₂ and CO. Inorganic Chemistry, 2020, 59, 4753-4763.	4.0	4
17	Spectroscopic and theoretical studies of UN and UN+. Journal of Chemical Physics, 2020, 152, 094302.	3.0	11
18	Guided Ion Beam and Quantum Chemical Investigation of the Thermochemistry of Thorium Dioxide Cations: Thermodynamic Evidence for Participation of f Orbitals in Bonding. Inorganic Chemistry, 2020, 59, 3118-3131.	4.0	16

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19	Coupled cluster spectroscopic properties of the coinage metal nitrosyls, Mâ€“NO (Mâ€‰=â€‰Cu, Ag, Au). Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
20	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	3.0	603
21	Beyond chemical accuracy in the heavy p-block: The first ionization potentials and electron affinities of Gaâ€“Kr, Inâ€“Xe, and Tlâ€“Rn. Journal of Chemical Physics, 2019, 151, 024303.	3.0	17
22	Bond energy of ThN+: A guided ion beam and quantum chemical investigation of the reactions of thorium cation with N2 and NO. Journal of Chemical Physics, 2019, 151, 034304.	3.0	20
23	Activation of Water by Pentavalent Actinide Dioxide Cations: Characteristic Curium Revealed by a Reactivity Turn after Americium. Inorganic Chemistry, 2019, 58, 14005-14014.	4.0	9
24	Potential Energy Surface of Group 11 Trimers (Cu, Ag, Au): Bond Angle Isomerism in Au3. Journal of Physical Chemistry A, 2019, 123, 1198-1207.	2.5	11
25	Solid Oganesson via a Many-Body Interaction Expansion Based on Relativistic Coupled-Cluster Theory and from Plane-Wave Relativistic Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 4201-4211.	2.5	23
26	Actinyl cationâ€“cation interactions in the gas phase: an accurate thermochemical study. Physical Chemistry Chemical Physics, 2019, 21, 7953-7964.	2.8	18
27	Gas Phase Hydrolysis and Oxoâ€Exchange of Actinide Dioxide Cations: Elucidating Intrinsic Chemistry from Protactinium to Einsteinium. Chemistry - A European Journal, 2019, 25, 4245-4254.	3.3	16
28	Electronic Structure Predictions of the Energetic Properties of Tellurium Fluorides. Inorganic Chemistry, 2019, 58, 8279-8292.	4.0	10
29	Computational Study of Molecular Hydrogen Adsorption over Small (MO₂)_n Nanoclusters (M = Ti, Zr, Hf; n = 1 to 4). Journal of Physical Chemistry A, 2018, 122, 4338-4349.	2.5	5
30	Alkali-Metal Trihalides: M+X3â€“Ion Pair or MXâ€“X2Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353.	2.6	8
31	Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds II: Fluorides, Chlorides, Oxides, and Hydroxides for Ba, Sr, and Ra. Journal of Physical Chemistry A, 2018, 122, 316-327.	2.5	18
32	On the Development of Accurate Gaussian Basis Sets for f-Block Elements. Annual Reports in Computational Chemistry, 2018, 14, 47-74.	1.7	6
33	Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: Hâ€“HÂ·Â·Â·Fâ€“M (M = Li,) Tj ETQq1 1 0.784314 rgBT Computation, 2018, 14, 5118-5127.	5.3	3
34	The photoelectron spectra of the isomeric 1- and 2-methyltetrazoles; their equilibrium structures and vibrational analysis by ab initio calculations. Journal of Chemical Physics, 2018, 149, 034305.	3.0	1
35	The bismuth tetramer Bi4: the Î½3 key to experimental observation. Physical Chemistry Chemical Physics, 2018, 20, 21881-21889.	2.8	3
36	Prediction of Bond Dissociation Energies/Heats of Formation for Diatomic Transition Metal Compounds: CCSD(T) Works. Journal of Chemical Theory and Computation, 2017, 13, 1057-1066.	5.3	92

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37	Acidity of M(VI)O2(OH)2 for M = Group 6, 16, and U as Central Atoms. Journal of Physical Chemistry A, 2017, 121, 1041-1050.	2.5	7
38	Benchmark-Quality Atomization Energies for BeH and BeH₂. Journal of Chemical Theory and Computation, 2017, 13, 649-653.	5.3	3
39	A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 084302.	3.0	3
40	Spectroscopic and theoretical studies of ThCl and ThCl+. Journal of Chemical Physics, 2017, 146, 054307.	3.0	10
41	A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 174301.	3.0	6
42	Remarkably High Stability of Late Actinide Dioxide Cations: Extending Chemistry to Pentavalent Berkelium and Californium. Chemistry - A European Journal, 2017, 23, 17369-17378.	3.3	19
43	Characterization of Carbenes via Hydrogenation Energies, Stability, and Reactivity: What's in a Name?. Chemistry - A European Journal, 2017, 23, 17556-17565.	3.3	11
44	Structural and Vibrational Properties of Iodopentafluorobenzene: A Combined Raman and Infrared Spectral and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 7917-7924.	2.5	3
45	The ionic states of difluoromethane: A reappraisal of the low energy photoelectron spectrum including ab initio configuration interaction computations. Journal of Chemical Physics, 2017, 147, 074305.	3.0	3
46	Correlation consistent basis sets for actinides. II. The atoms Ac and Npâ€“Lr. Journal of Chemical Physics, 2017, 147, 084108.	3.0	63
47	Guided ion beam and theoretical studies of the bond energy of SmS+. Journal of Chemical Physics, 2017, 147, 214307.	3.0	5
48	Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification. Journal of Chemical Physics, 2017, 147, 024302.	3.0	4
49	Gaussian basis sets for use in correlated molecular calculations. XI. Pseudopotential-based and all-electron relativistic basis sets for alkali metal (Kâ€“Fr) and alkaline earth (Caâ€“Ra) elements. Journal of Chemical Physics, 2017, 147, 244106.	3.0	144
50	A combined photoelectron spectroscopy and relativistic ab initio studies of the electronic structures of UFO and UFOâ¯. Journal of Chemical Physics, 2016, 144, 084309.	3.0	4
51	Ab initio ro-vibronic spectroscopy of the Î2 PCS radical and Î£+1PCSâ¯ anion. Journal of Chemical Physics, 2016, 145, 224303.	3.0	5
52	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene. Journal of Chemical Physics, 2016, 144, 124302.	3.0	11
53	A spectroscopic case for SPSi detection: The third-row in a single molecule. Journal of Chemical Physics, 2016, 145, 124311.	3.0	41
54	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. Journal of Chemical Physics, 2016, 144, 214101.	3.0	89

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55	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene. Journal of Chemical Physics, 2016, 144, 204305.	3.0	15
56	Correlation consistent basis sets for lanthanides: The atoms Laâ€“Lu. Journal of Chemical Physics, 2016, 145, 054111.	3.0	96
57	Bond energies of ThO+ and ThC+: A guided ion beam and quantum chemical investigation of the reactions of thorium cation with O2 and CO. Journal of Chemical Physics, 2016, 144, 184309.	3.0	48
58	Use of Improved Orbitals for CCSD(T) Calculations for Predicting Heats of Formation of Group IV and Group VI Metal Oxide Monomers and Dimers and UCl₆. Journal of Chemical Theory and Computation, 2016, 12, 3583-3592.	5.3	43
59	Structures and Properties of the Products of the Reaction of Lanthanide Atoms with H₂O: Dominance of the +II Oxidation State. Journal of Physical Chemistry A, 2016, 120, 793-804.	2.5	15
60	Theoretical spectroscopy study of the low-lying electronic states of UX and UX+, X = F and Cl. Journal of Chemical Physics, 2015, 143, 184313.	3.0	17
61	Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations. Journal of Chemical Physics, 2015, 143, 164303.	3.0	19
62	Multireference configuration interaction calculations of the first six ionization potentials of the uranium atom. Journal of Chemical Physics, 2015, 143, 184308.	3.0	10
63	Correlation consistent basis sets for actinides. I. The Th and U atoms. Journal of Chemical Physics, 2015, 142, 074105.	3.0	135
64	Reliable Potential Energy Surfaces for the Reactions of H₂O with ThO₂, PaO₂⁺, UO₂²⁺, and UO₂⁺. Journal of Physical Chemistry A, 2015, 119, 11422-11431.	2.5	55
65	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	26
66	Gas Phase Properties of MX₂ and MX₄ (X = F, Cl) for M = Group 4, Group 14, Cerium, and Thorium. Journal of Physical Chemistry A, 2015, 119, 5790-5803.	2.5	43
67	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. Molecular Physics, 2015, 113, 1551-1558.	1.7	57
68	Accurate Calculation of the Dissociation Energy of the Highly Anharmonic System ClHCl^{â€“}. Journal of Physical Chemistry A, 2015, 119, 5158-5164.	2.5	4
69	Composite thermochemistry of gas phase U(VI)-containing molecules. Journal of Chemical Physics, 2014, 141, 244308.	3.0	28
70	Static electric dipole polarizabilities of An5+/6+ and AnO2+/2+ (An = U, Np, and Pu) ions. Journal of Chemical Physics, 2014, 141, 234304.	3.0	4
71	Ab initio ro-vibronic spectroscopy of SiCCl ($ilde{X}^2Pi$Xì f2î). Journal of Chemical Physics, 2014, 141, 034305.	3.0	4
72	A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. Journal of Chemical Physics, 2014, 141, 104302.	3.0	41

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73	Correlation consistent basis sets for explicitly correlated wavefunctions: Pseudopotential-based basis sets for the post-d main group elements Gaâ€“Rn. Journal of Chemical Physics, 2014, 141, 094106.	3.0	62
74	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. Theoretical Chemistry Accounts, 2014, 133, .	1.4	72
75	Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	95
76	Correlation consistent, Douglasâ€“Krollâ€“Hess relativistic basis sets for the 5p and 6p elements. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	60
77	Reactions of Lanthanide Atoms with Oxygen Difluoride and the Role of the Ln Oxidation State. Inorganic Chemistry, 2014, 53, 446-456.	4.0	25
78	Experimental and theoretical investigation of correlated fine structure branching ratios arising from state-selected predissociation of BrO (A²Î_{3/2}). Physical Chemistry Chemical Physics, 2014, 16, 607-615.	2.8	1
79	An ab initio investigation of the ground and low-lying singlet and triplet electronic states of XNO2 and XONO (X = Cl, Br, and I). Journal of Chemical Physics, 2014, 140, 044308.	3.0	5
80	An expanded calibration study of the explicitly correlated CCSD(T)-F12b method using large basis set standard CCSD(T) atomization energies. Journal of Chemical Physics, 2013, 139, 084110.	3.0	48
81	Explicitly correlated composite thermochemistry of transition metal species. Journal of Chemical Physics, 2013, 139, 094302.	3.0	79
82	Accurate bond dissociation energies (D0) for FHFâ¯isotopologues. Molecular Physics, 2013, 111, 2647-2652.	1.7	17
83	Correlation Consistent Gaussian Basis Sets for H, Bâ€“Ne with Diracâ€“Fock AREP Pseudopotentials: Applications in Quantum Monte Carlo Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2170-2178.	5.3	27
84	Is near-â€œspectroscopic accuracyâ€•possible for heavy atoms and coupled cluster theory? An investigation of the first ionization potentials of the atoms Gaâ€“Kr. Journal of Chemical Physics, 2013, 138, 164312.	3.0	7
85	Anharmonic zero point vibrational energies: Tipping the scales in accurate thermochemistry calculations?. Journal of Chemical Physics, 2013, 138, 044311.	3.0	52
86	Thermal Rate Constants for the O(³P) + HBr and O(³P) + DBr Reactions: Transition-State Theory and Quantum Mechanical Calculations. Journal of Physical Chemistry A, 2013, 117, 12703-12710.	2.5	6
87	Static Electric Dipole Polarizabilities of Tri- and Tetravalent U, Np, and Pu Ions. Journal of Physical Chemistry A, 2013, 117, 11874-11880.	2.5	3
88	The alkaline earth dimer cations (Be₂ ⁺, Mg₂ ⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Coupled cluster and full configuration interaction studies^{â€}. Molecular Physics, 2013, 111, 2292-2298.	1.7	54
89	Ab initio ro-vibrational spectroscopy of the group 11 cyanides: CuCN, AgCN, and AuCN. Journal of Chemical Physics, 2013, 138, 134314.	3.0	25
90	State-Selected Reaction of Muonium with Vibrationally Excited H₂. Journal of Physical Chemistry Letters, 2012, 3, 2755-2760.	4.6	24

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91	The Use of Explicitly Correlated Methods on XeF₆ Predicts a C_{3v} Minimum with a Sterically Active, Free Valence Electron Pair on Xe. Journal of Physical Chemistry A, 2012, 116, 9777-9782.	2.5	29
92	Spectroscopic investigations of ThF and ThF+. Journal of Chemical Physics, 2012, 136, 104305.	3.0	36
93	Accurate ab initio potential energy surfaces for the 3Aâ€²â€² and 3Aâ€² electronic states of the O(3P)+HBr system. Journal of Chemical Physics, 2012, 136, 174316.	3.0	8
94	A Practical Guide to Reliable First Principles Computational Thermochemistry Predictions Across the Periodic Table. Annual Reports in Computational Chemistry, 2012, , 1-28.	1.7	94
95	Explicitly Correlated Coupled Cluster Calculations for Molecules Containing Group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) Elements: Optimized Complementary Auxiliary Basis Sets for Valence and Coreâ€“Valence Basis Sets. Journal of Chemical Theory and Computation, 2012, 8, 518-526.	5.3	39
96	Further benchmarks of a composite, convergent, statistically calibrated coupled-cluster-based approach for thermochemical and spectroscopic studies. Molecular Physics, 2012, 110, 2381-2399.	1.7	170
97	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	381
98	Are ab initio quantum chemistry methods able to predict vibrational states up to the dissociation limit for multi-electron molecules close to spectroscopic accuracy?. Physical Chemistry Chemical Physics, 2011, 13, 3654-3659.	2.8	19
99	Ab Initio Coupled Cluster Determination of the Heats of Formation of C₂H₂F₂, C₂F₂, and C₂F₄. Journal of Physical Chemistry A, 2011, 115, 1440-1451.	2.5	38
100	Accurate ab initio ro-vibronic spectroscopy of the $ilde X^2 Pi$XÌƒ2Î CCN radical using explicitly correlated methods. Journal of Chemical Physics, 2011, 135, 144309.	3.0	29
101	On the effectiveness of CCSD(T) complete basis set extrapolations for atomization energies. Journal of Chemical Physics, 2011, 135, 044102.	3.0	250
102	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.	1.4	536
103	Accurate potential energy curves for the group 12 dimers Zn2, Cd2, and Hg2. Theoretical Chemistry Accounts, 2011, 129, 651-656.	1.4	33
104	Application of explicitly correlated coupled-cluster methods to molecules containing post-3d main group elements. Molecular Physics, 2011, 109, 2607-2623.	1.7	33
105	Kinetic Isotope Effects for the Reactions of Muonic Helium and Muonium with H ₂. Science, 2011, 331, 448-450.	12.6	86
106	Ab initio spectroscopic characterization of the HNNO and ONHN radicals. Journal of Chemical Physics, 2011, 134, 084308.	3.0	11
107	The kinetics study of the S + S2â†' S3reaction by the chaperone mechanism. Journal of Chemical Physics, 2011, 134, 154508.	3.0	7
108	Kinetics of the reaction of the heaviest hydrogen atom with H2, the 4HeÎ¼Â+ÂH2 â†' 4HeÎ¼H +ÂH reaction: Experiments, accurate quantal calculations, and variational transition state theory, including kinetic isotope effects for a factor of 36.1 in isotopic mass. Journal of Chemical Physics, 2011, 135, 184310.	3.0	35

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109	Third Row Transition Metal Hexafluorides, Extraordinary Oxidizers, and Lewis Acids: Electron Affinities, Fluoride Affinities, and Heats of Formation of WF₆, ReF₆, OsF₆, IrF₆, PtF₆, and AuF₆. Inorganic Chemistry, 2010, 49, 1056-1070.	4.0	109
110	A highly accurate potential energy curve for the mercury dimer. Journal of Chemical Physics, 2010, 132, 114301.	3.0	43
111	Molecular core-valence correlation effects involving the post-d elements Gaâ€“Rn: Benchmarks and new pseudopotential-based correlation consistent basis sets. Journal of Chemical Physics, 2010, 133, 174116.	3.0	207
112	Structures and Heats of Formation of Simple Alkali Metal Compounds: Hydrides, Chlorides, Fluorides, Hydroxides, and Oxides for Li, Na, and K. Journal of Physical Chemistry A, 2010, 114, 4272-4281.	2.5	37
113	Refined Theoretical Estimates of the Atomization Energies and Molecular Structures of Selected Small Oxygen Fluorides. Journal of Physical Chemistry A, 2010, 114, 613-623.	2.5	36
114	A theoretical study of the low-lying electronic states of OIO and the ground states of IOO and OIO^{â^’}. Molecular Physics, 2010, 108, 393-408.	1.7	19
115	Thermodynamic Properties of the XO₂, X₂O, XYO, X₂O₂, and XYO₂ (X, Y = Cl, Br, and I) Isomers. Journal of Physical Chemistry A, 2010, 114, 4254-4265.	2.5	38
116	Calibration study of the CCSD(T)-F12a/b methods for C2 and small hydrocarbons. Journal of Chemical Physics, 2010, 133, 184102.	3.0	57
117	Correlation consistent basis sets for molecular core-valence effects with explicitly correlated wave functions: The atoms Bâ€“Ne and Alâ€“Ar. Journal of Chemical Physics, 2010, 132, 054108.	3.0	253
118	Correlation consistent basis sets for explicitly correlated wavefunctions: valence and coreâ€“valence basis sets for Li, Be, Na, and Mg. Physical Chemistry Chemical Physics, 2010, 12, 10460.	2.8	104
119	Functional Representation for the Bornâ^’Oppenheimer Diagonal Correction and Bornâ^’Huang Adiabatic Potential Energy Surfaces for Isotopomers of H₃. Journal of Physical Chemistry A, 2009, 113, 4479-4488.	2.5	34
120	High level coupled cluster determination of the structure, frequencies, and heat of formation of water. Journal of Chemical Physics, 2009, 131, 154306.	3.0	34
121	Optimized complementary auxiliary basis sets for explicitly correlated methods: aug-cc-pVnZ orbital basis sets. Chemical Physics Letters, 2009, 476, 303-307.	2.6	196
122	Accurate Thermochemistry for Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2009, 113, 7861-7877.	2.5	156
123	Energy-Consistent Pseudopotentials for the 5d Elementsâ€”Benchmark Calculations for Oxides, Nitrides, and Pt₂. Journal of Physical Chemistry A, 2009, 113, 12478-12484.	2.5	16
124	Extrapolating MP2 and CCSD explicitly correlated correlation energies to the complete basis set limit with first and second row correlation consistent basis sets. Journal of Chemical Physics, 2009, 131, 194105.	3.0	251
125	On the Ionization Energy of HfO. Journal of Physical Chemistry A, 2009, 113, 12353-12355.	2.5	6
126	Energy-consistent pseudopotentials and correlation consistent basis sets for the 5d elements Hfâ€“Pt. Journal of Chemical Physics, 2009, 130, 164108.	3.0	579

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127	Does the 4f Electron Configuration Affect Molecular Geometries? A Joint Computational, Vibrational Spectroscopic, and Electron Diffraction Study of Dysprosium Tribromide. Inorganic Chemistry, 2009, 48, 4143-4153.	4.0	16
128	Heats of Formation of the H1,2OmSn (m, n = 0â^'3) Molecules from Electronic Structure Calculations. Journal of Physical Chemistry A, 2009, 113, 11343-11353.	2.5	52
129	A theoretical study of the spectroscopic properties of the ground and first excited electronic state of HS2. Chemical Physics, 2008, 346, 34-44.	1.9	29
130	A survey of factors contributing to accurate theoretical predictions of atomization energies and molecular structures. Journal of Chemical Physics, 2008, 129, 204105.	3.0	345
131	ClClO2 Is the Most Stable Isomer of Cl2O2. Accurate Coupled Cluster Energetics and Electronic Spectra of Cl2O2 Isomers. Journal of Physical Chemistry A, 2008, 112, 9623-9627.	2.5	24
132	Benchmark calculations on the adiabatic ionization potentials of Mâ€“NH3â€^(M=Na,Al,Ga,In,Cu,Ag). Journal of Chemical Physics, 2008, 128, 154301.	3.0	16
133	Structure and Heats of Formation of Iodine Fluorides and the Respective Closed-Shell Ions from CCSD(T) Electronic Structure Calculations and Reliable Prediction of the Steric Activity of the Free-Valence Electron Pair in ClF₆^{â^'}, BrF₆^{â^'}, and IF₆^{â^'}. Inorganic Chemistry, 2008, 47, 5485-5494.	4.0	53
134	Optimized auxiliary basis sets for explicitly correlated methods. Journal of Chemical Physics, 2008, 129, 184108.	3.0	445
135	Prediction of Vibrational Frequencies of UO22+ at the CCSD(T) Level. Journal of Physical Chemistry A, 2008, 112, 4095-4099.	2.5	45
136	The CCSD(T) complete basis set limit for Ne revisited. Journal of Chemical Physics, 2008, 129, 194115.	3.0	41
137	Systematically convergent basis sets for explicitly correlated wavefunctions: The atoms H, He, Bâ€“Ne, and Alâ€“Ar. Journal of Chemical Physics, 2008, 128, 084102.	3.0	1,115
138	Determination of the rate constant for sulfur recombination by quasiclassical trajectory calculations. Journal of Chemical Physics, 2008, 128, 204306.	3.0	22
139	Probing the limits of accuracy in electronic structure calculations: Is theory capable of results uniformly better than â€œchemical accuracyâ€?. Journal of Chemical Physics, 2007, 126, 114105.	3.0	87
140	Hg+Brâ†'HgBr recombination and collision-induced dissociation dynamics. Journal of Chemical Physics, 2007, 127, 164304.	3.0	47
141	Chapter 11 Gaussian Basis Sets Exhibiting Systematic Convergence to the Complete Basis Set Limit. Annual Reports in Computational Chemistry, 2007, 3, 195-206.	1.7	49
142	Correlation Consistent Basis Sets with Relativistic Effective Core Potentials: The Transition Metal Elements Y and Hg. ACS Symposium Series, 2007, , 125-151.	0.5	2
143	Energy-consistent relativistic pseudopotentials and correlation consistent basis sets for the 4d elements Yâ€“Pd. Journal of Chemical Physics, 2007, 126, 124101.	3.0	822
144	Aqueous Microsolvation of Mercury Halide Speciesâ€. Journal of Physical Chemistry A, 2007, 111, 11342-11349.	2.5	28

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145	The group 12 metal chalcogenides: an accurate multireference configuration interaction and coupled cluster study. Molecular Physics, 2007, 105, 1139-1155.	1.7	61
146	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.	2.5	138
147	Heats of Formation of Krypton Fluorides and Stability Predictions for KrF₄ and KrF₆ from High Level Electronic Structure Calculations. Inorganic Chemistry, 2007, 46, 10016-10021.	4.0	25
148	Quantitative Computational Thermochemistry of Transition Metal Species. Journal of Physical Chemistry A, 2007, 111, 11269-11277.	2.5	153
149	The Nature of HalogenÂ·Â·Â·Halide Synthons:â€‰ Theoretical and Crystallographic Studies. Journal of Physical Chemistry A, 2007, 111, 2319-2328.	2.5	78
150	Coupled-cluster study of the electronic structure and energetics of tetrasulfur, S4. Journal of Chemical Physics, 2007, 127, 174305.	3.0	23
151	Chemically Accurate Thermochemistry of Cadmium:â€‰ An ab Initio Study of Cd + XY (X = H, O, Cl, Br; Y =) Tj ETQq1 1 0.784314 rgBT	2.5	26
152	On the Spectroscopic and Thermochemical Properties of ClO, BrO, IO, and Their Anions. Journal of Physical Chemistry A, 2006, 110, 13877-13883.	2.5	706
153	Comment on â€˜Pople versus Dunning basis sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standardâ€™ by R.A. Klein and M.A. Zottola [Chem. Phys. Lett. 419 (2006) 254â€“258]. Chemical Physics Letters, 2006, 430, 459-463.	2.6	7
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