David A Dixon

List of Publications by Year
in descending order

188 papers	4,650 citations	101384 36 h-index	133063 59 g-index
195 all docs	195 docs citations	195 times ranked	5473 citing authors

#	Article	IF	Citations
1	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	381
2	Atomically dispersed supported metal catalysts: perspectives and suggestions for future research. Catalysis Science and Technology, 2017, 7, 4259-4275.	2.1	221
3	Thermodynamic Properties of Molecular Borane Amines and the [BH4-][NH4+] Salt for Chemical Hydrogen Storage Systems from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2005, 109, 5129-5135.	1.1	198
4	Further benchmarks of a composite, convergent, statistically calibrated coupled-cluster-based approach for thermochemical and spectroscopic studies. Molecular Physics, 2012, 110, 2381-2399.	0.8	170
5	Unusual structure, bonding and properties in a californium borate. Nature Chemistry, 2014, 6, 387-392.	6.6	110
6	Emergence of californium as the second transitional element in the actinide series. Nature Communications, 2015, 6, 6827.	5.8	108
7	The Least Stable Isomer of BN Naphthalene: Toward Predictive Trends for the Optoelectronic Properties of BN Acenes. Journal of the American Chemical Society, 2017, 139, 6082-6085.	6.6	100
8	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 12609-12616.	7.2	96
9	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.	2.3	92
10	Electrochemical Conversion of Muconic Acid to Biobased Diacid Monomers. ACS Sustainable Chemistry and Engineering, 2016, 4, 3575-3585.	3.2	81
11	Late-Stage Functionalization of 1,2-Dihydro-1,2-azaborines via Regioselective Iridium-Catalyzed Câ€“H Borylation: The Development of a New N,N-Bidentate Ligand Scaffold. Journal of the American Chemical Society, 2015, 137, 5536-5541.	6.6	80
12	Heats of Formation of Xenon Fluorides and the Fluxionality of XeF6from High Level Electronic Structure Calculations. Journal of the American Chemical Society, 2005, 127, 8627-8634.	6.6	75
13	Tree Growthâ€"Hybrid Genetic Algorithm for Predicting the Structure of Small (TiO₂)_n, n = 2â€“13, Nanoclusters. Journal of Chemical Theory and Computation, 2013, 9, 3189-3200.	2.3	71
14	Prediction of the pK_aâ€™s of Aqueous Metal Ion +2 Complexes. Journal of Physical Chemistry A, 2015, 119, 2926-2939.	1.1	67
15	BN-substituted diphenylacetylene: a basic model for conjugated Ï€-systems containing the BN bond pair. Chemical Science, 2012, 3, 825-829.	3.7	66
16	Gold Nanorod-Enhanced Light Absorption and Photoelectrochemical Performance of Î±-Fe₂O₃ Thin-Film Electrode for Solar Water Splitting. Journal of Physical Chemistry C, 2013, 117, 22060-22068.	1.5	65
17	Beating Heterogeneity of Single-Site Catalysts: MgO-Supported Iridium Complexes. ACS Catalysis, 2018, 8, 3489-3498.	5.5	64
18	Perfluoroalkyl Cobalt(III) Fluoride and Bis(perfluoroalkyl) Complexes: Catalytic Fluorination and Selective Difluorocarbene Formation. Journal of the American Chemical Society, 2015, 137, 16064-16073.	6.6	63

#	Article	IF	Citations
19	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	1.5	62
20	Substituent Effects on the Properties of Borafluorenes. Organometallics, 2016, 35, 3182-3191.	1.1	58
21	Reliable Potential Energy Surfaces for the Reactions of H₂O with ThO₂, PaO₂⁺, UO₂²⁺, and UO₂⁺. Journal of Physical Chemistry A, 2015, 119, 11422-11431.	1.1	55
22	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.	1.9	53
23	Prototype Supported Metal Cluster Catalysts: Ir₄ and Ir₆. ChemCatChem, 2011, 3, 95-107.	1.8	53
24	Selective molecular recognition by nanoscale environments in a supported iridium cluster catalyst. Nature Nanotechnology, 2014, 9, 459-465.	15.6	53
25	Structural and Electronic Property Study of (ZnO)_n, n â‰ 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 20400-20418.	1.5	53
26	Investigation of the Structure and Active Sites of TiO₂ Nanorod Supported VO_x Catalysts by High-Field and Fast-Spinning ⁵¹V MAS NMR. ACS Catalysis, 2015, 5, 3945-3952.	5.5	51
27	A Modular Synthetic Approach to Monocyclic 1,4â€Azaborines. Angewandte Chemie - International Edition, 2016, 55, 8333-8337.	7.2	50
28	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie - International Edition, 2015, 54, 7823-7827.	7.2	49
29	Accurate Heats of Formation of the â€œArduengo-Typeâ€•Carbene and Various Adducts Including H2 from ab Initio Molecular Orbital Theory. Journal of Physical Chemistry A, 2006, 110, 1968-1974.	1.1	48
30	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie, 2019, 131, 12739-12746.	1.6	45
31	Formation Mechanisms and Defect Engineering of Imine-Based Porous Organic Cages. Chemistry of Materials, 2018, 30, 262-272.	3.2	44
32	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.	1.1	43
33	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.	2.3	43
34	Molecular and Dissociative Adsorption of Water on (TiO₂)_n Clusters, n = 1â€“4. Journal of Physical Chemistry A, 2015, 119, 11406-11421.	1.1	39
35	Investigation of Silica-Supported Vanadium Oxide Catalysts by High-Field ⁵¹V Magic-Angle Spinning NMR. Journal of Physical Chemistry C, 2017, 121, 6246-6254.	1.5	39
36	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO₂. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791.	4.0	38

#	Article	IF	Citations
37	Electrochemical and Spectroscopic Properties of Boron Dipyrromethene–Thiophene–Triphenylamine-Based Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2016, 120, 9068-9080.	1.5	36
38	High–Energy–Resolution X–ray Absorption Spectroscopy for Identification of Reactive Surface Species on Supported Single–Site Iridium Catalysts. Chemistry - A European Journal, 2017, 23, 14760-14768.	1.7	35
39	Are DTTO and iso–DTTO Worthwhile Targets for Synthesis?. Propellants, Explosives, Pyrotechnics, 2015, 40, 463-468.	1.0	34
40	Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3689-3710.	2.3	32
41	Methyl Cation Affinities of Rare Gases and Nitrogen and the Heat of Formation of Diazomethane. Journal of Physical Chemistry A, 2005, 109, 4073-4080.	1.1	31
42	Reversible Metal Aggregation and Redispersion Driven by the Catalytic Water Gas Shift Half-Reactions: Interconversion of Single-Site Rhodium Complexes and Tetrarhodium Clusters in Zeolite HY. ACS Catalysis, 2019, 9, 3311-3321.	5.5	31
43	Role of Electronegative Substituents on the Bond Energies in the Grubbs Metathesis Catalysts for M = Fe, Ru, Os. Journal of Physical Chemistry C, 2014, 118, 13563-13577.	1.5	30
44	Thermochemical Properties of HxNO Molecules and Ions from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2006, 110, 185-191.	1.1	28
45	Mechanism of selective and complete oxidation in La₂O₃-catalyzed oxidative coupling of methane. Catalysis Science and Technology, 2020, 10, 2602-2614.	2.1	28
46	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.	1.9	25
47	Single–Site Zeolite–Anchored Organoiridium Carbonyl Complexes: Characterization of Structure and Reactivity by Spectroscopy and Computational Chemistry. Chemistry - A European Journal, 2015, 21, 11825-11835.	1.7	25
48	Dynamics of Magnesite Formation at Low Temperature and High pCO₂ in Aqueous Solution. Environmental Science & Technology, 2015, 49, 10736-10744.	4.6	25
49	MgO-Supported Iridium Metal Pair-Site Catalysts Are More Active and Resistant to CO Poisoning than Analogous Single-Site Catalysts for Ethylene Hydrogenation and Hydrogen–Deuterium Exchange. ACS Catalysis, 2019, 9, 9545-9553.	5.5	25
50	Predictive Acid Gas Adsorption in Rare Earth DOBDC Metal–Organic Frameworks via Complementary Cluster and Periodic Structure Models. Journal of Physical Chemistry C, 2020, 124, 26801-26813.	1.5	25
51	Properties of Cerium Hydroxides from Matrix Infrared Spectra and Electronic Structure Calculations. Inorganic Chemistry, 2016, 55, 1702-1714.	1.9	24
52	Acid Gas Adsorption on Metal–Organic Framework Nanosheets as a Model of an “All-Surface” Material. Journal of Chemical Theory and Computation, 2017, 13, 1341-1350.	2.3	23
53	Infrared Spectra and Quantum Chemical Calculations of the Bridge-Bonded HC(F)LnF₂ (Ln) Tj ETQq1 1 0.784314 rgBT /O	1.1	22
54	The Synthesis, Characterization and Dehydrogenation of Sigma–Complexes of BN–Cyclohexanes. Chemistry - A European Journal, 2016, 22, 310-322.	1.7	22

#	Article	IF	Citations
55	Initial Steps in the Selective Catalytic Reduction of NO with NH₃ by TiO₂-Supported Vanadium Oxides. ACS Catalysis, 2020, 10, 13918-13931.	5.5	22
56	Uranium(IV) Chloride Complexes: UCl₆^{2â€“} and an Unprecedented U(H₂O)₄Cl₄ Structural Unit. Inorganic Chemistry, 2017, 56, 9772-9780.	1.9	21
57	Surface-Catalyzed Oxygen Exchange during Mineral Carbonation in Nanoscale Water Films. Journal of Physical Chemistry C, 2019, 123, 12871-12885.	1.5	21
58	Formation of Surface Impurities on Lithiumâ€“Nickelâ€“Manganeseâ€“Cobalt Oxides in the Presence of CO₂ and H₂O. Journal of the American Chemical Society, 2021, 143, 10261-10274.	6.6	21
59	Formation and Characterization of Homoleptic Thorium Isocyanide Complexes. Inorganic Chemistry, 2017, 56, 5060-5068.	1.9	20
60	Remarkably High Stability of Late Actinide Dioxide Cations: Extending Chemistry to Pentavalent Berkelium and Californium. Chemistry - A European Journal, 2017, 23, 17369-17378.	1.7	19
61	How Energetic are cycloâ€Pentazolates?. Propellants, Explosives, Pyrotechnics, 2019, 44, 263-266.	1.0	19
62	Structures and Energetics of (MgCO₃)_n Clusters (n â‰¤ 16). Journal of Physical Chemistry A, 2015, 119, 3419-3428.	1.1	18
63	Singleâ€Site Osmium Catalysts on MgO: Reactivity and Catalysis of CO Oxidation. Chemistry - A European Journal, 2017, 23, 2532-2536.	1.7	18
64	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.	1.1	18
65	Structure and Stability of Hydrolysis Reaction Products of MgO Nanoparticles Leading to the Formation of Brucite. Journal of Physical Chemistry C, 2017, 121, 21750-21762.	1.5	17
66	Metal Heptafluoroisopropyl (M-hfip) Complexes for Use as hfip Transfer Agents. Organometallics, 2018, 37, 422-432.	1.1	17
67	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.	1.9	17
68	Time-Dependent Density Functional Theory Predictions of the Vertical Excitation Energies of Silanones as Models for the Excitation Process in Porous Silicon. Journal of Physical Chemistry B, 2005, 109, 14830-14835.	1.2	16
69	Reaction of Laser-Ablated Uranium and Thorium Atoms with H₂Se: A Rare Example of Selenium Multiple Bonding. Inorganic Chemistry, 2015, 54, 9761-9769.	1.9	16
70	Water Structure Controls Carbonic Acid Formation in Adsorbed Water Films. Journal of Physical Chemistry Letters, 2018, 9, 4988-4994.	2.1	16
71	Understanding the Binding of Aromatic Hydrocarbons on Rutile TiO₂(110). Journal of Physical Chemistry C, 2019, 123, 16766-16777.	1.5	16
72	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.	1.7	16

#	Article	IF	Citations
73	Accelerating the insertion reactions of (NHC)Cuâ€“H via remote ligand functionalization. Chemical Science, 2021, 12, 11495-11505.	3.7	16
74	Shiftâ€andâ€invert parallel spectral transformation eigensolver: Massively parallel performance for densityâ€functional based tightâ€binding. Journal of Computational Chemistry, 2016, 37, 448-459.	1.5	15
75	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.	1.1	15
76	Density Functional Theory and the Basis Set Truncation Problem with Correlation Consistent Basis Sets: Elephant in the Room or Mouse in the Closet?. Journal of Physical Chemistry A, 2018, 122, 2598-2603.	1.1	15
77	Experimental and Theoretical Studies of the Photoreduction of Copper(II)â^Dendrimer Complexes. Journal of Physical Chemistry C, 2008, 112, 1335-1344.	1.5	14
78	The Vanadium(V) Oxoazides [VO(N₃)₃], [(bipy)VO(N₃)₃], and [VO(N₃)₅]^{2â^}. Angewandte Chemie - International Edition, 2015, 54, 9101-9105.	7.2	14
79	Structures and Stabilities of (CaO)_n Nanoclusters. Journal of Physical Chemistry C, 2017, 121, 23025-23038.	1.5	14
80	The Uranium(VI) Oxoazides [UO₂(N₃)₂â‹…CH₃CN], [(bipy)₂(UO₂)₂(N₃)₄], [(bipy)UO₂(N₃)₃]^{â^}, [UO₂(N₃)₄]^{2â^}, and [(UO₂)₂(N₃)₈]^{4â^}. Chemistry - A European Journal, 2017, 23, 652-664.	1.7	14
81	Synthesis of 1H-Pyrazol-5-yl-pyridin-2-yl-[1,2,4]triazinyl Soft-Lewis Basic Complexants via Metal and Oxidant Free [3 + 2] Dipolar Cycloaddition of Terminal Ethynyl Pyridines with Tosylhydrazides. Journal of Organic Chemistry, 2019, 84, 14558-14570.	1.7	14
82	Tetrakis(ethylmethylamido) Hafnium Adsorption and Reaction on Hydrogen-Terminated Si(100) Surfaces. Journal of Physical Chemistry C, 2011, 115, 18560-18571.	1.5	13
83	Prediction of the Thermodynamic Properties of Key Products and Intermediates from Biomass. II. Journal of Physical Chemistry C, 2012, 116, 20738-20754.	1.5	13
84	An Experimental and Computational Study of the Gas-Phase Acidities of the Common Amino Acid Amides. Journal of Physical Chemistry B, 2015, 119, 9661-9669.	1.2	13
85	Reaction of CO₂ with Groups 4 and 6 Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2017, 121, 8719-8727.	1.1	13
86	The Molybdenum(V) and Tungsten(VI) Oxoazides [MoO(N₃)₃], [MoO(N₃)₃â‹…2â€‰CH₃CN], [(bipy)MoO(N₃)₃], [MoO(N₃)₅]^{2â^}, [WO(N₃)₄], and [WO(N₃)₄â‹…CH₃CN]. Angewandte Chemie - International Edition, 2015, 54, 15550-15555.	7.2	12
87	Preparation and Characterization of Antimony and Arsenic Tricyanide and Their 2,2â€²â€Bipyridine Adducts. Chemistry - A European Journal, 2016, 22, 13251-13257.	1.7	12
88	Extending the Row of Lanthanide Tetrafluorides: A Combined Matrixâ€Isolation and Quantumâ€Chemical Study. Chemistry - A European Journal, 2016, 22, 2406-2416.	1.7	12
89	Laser-Ablated U Atom Reactions with (CN)₂ to Form UNC, U(NC)₂, and U(NC)₄: Matrix Infrared Spectra and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2018, 122, 516-528.	1.1	12
90	Machine-Learning Approach for the Development of Structureâ€“Energy Relationships of ZnO Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 18621-18639.	1.5	12

#	Article	IF	Citations
91	Monomeric and Trimeric Thorium Chlorides Isolated from Acidic Aqueous Solution. Inorganic Chemistry, 2019, 58, 10871-10882.	1.9	12
92	Solubility thermodynamics of amine boranes in polar solvents. International Journal of Hydrogen Energy, 2021, 46, 10801-10808.	3.8	12
93	The Binary Groupâ€...4 Azides [PPh₄]₂[Zr(N₃)₆] and [PPh₄]₂[Hf(N₃)₆]. Angewandte Chemie - International Edition, 2016, 55, 14350-14354.	7.2	11
94	Thorium and Uranium Hydride Phosphorus and Arsenic Bearing Molecules with Single and Double Actinide-Pnictogen and Bridged Agostic Hydrogen Bonds. Inorganic Chemistry, 2017, 56, 2949-2957.	1.9	11
95	Properties of Lanthanide Hydroxide Molecules Produced in Reactions of Lanthanide Atoms with H₂O₂ and H₂ + O₂ Mixtures: Roles of the +I, +II, +III, and +IV Oxidation States. Journal of Physical Chemistry A, 2017, 121, 1779-1796.	1.1	11
96	Characterization of Carbenes via Hydrogenation Energies, Stability, and Reactivity: What's in a Name?. Chemistry - A European Journal, 2017, 23, 17556-17565.	1.7	11
97	Potential Energy Surface of Group 11 Trimers (Cu, Ag, Au): Bond Angle Isomerism in Au3. Journal of Physical Chemistry A, 2019, 123, 1198-1207.	1.1	11
98	Energetics of CO2â€“ in Aqueous Solution. Journal of Physical Chemistry A, 2019, 123, 1243-1259.	1.1	11
99	Lewis Acidity and Basicity: Another Measure of Carbene Reactivity. Journal of Physical Chemistry A, 2020, 124, 6096-6103.	1.1	11
100	Elucidation of Bottom-Up Growth of CaCO₃ Involving Prenucleation Clusters from Structure Predictions and Decomposition of Globally Optimized (CaCO₃)_n Nanoclusters. ACS Nano, 2020, 14, 4153-4165.	7.3	11
101	Nature of Oxygen Adsorption on Defective Carbonaceous Materials. Journal of Physical Chemistry C, 2021, 125, 20686-20696.	1.5	11
102	Formation Mechanism of NF₄⁺ Salts and Extraordinary Enhancement of the Oxidizing Power of Fluorine by Strong Lewis Acids. Angewandte Chemie - International Edition, 2017, 56, 7924-7929.	7.2	10
103	Thermodynamic Acidity Studies of 6,6â€²-Dihydroxy-2,2â€²-bipyridine: A Combined Experimental and Computational Approach. Journal of Physical Chemistry A, 2018, 122, 2221-2231.	1.1	10
104	Electronic Structure Predictions of the Energetic Properties of Tellurium Fluorides. Inorganic Chemistry, 2019, 58, 8279-8292.	1.9	10
105	The Hâ€¢/H^{â€“} Redox Couple and Absolute Hydration Energy of H^{â€“}. Journal of Physical Chemistry A, 2020, 124, 6084-6095.	1.1	10
106	Prediction of Structures and Atomization Energies of Coinage Metals, (M)_n, n < 20: Extrapolation of Normalized Clustering Energies to Predict the Cohesive Energy. Journal of Physical Chemistry A, 2020, 124, 1775-1786.	1.1	10
107	Bond Dissociation Energies in Heavy Element Chalcogen and Halogen Small Molecules. Journal of Physical Chemistry A, 2021, 125, 1892-1902.	1.1	10
108	Structures and Stability of Irn(CO)m. Molecular Physics, 2012, 110, 1977-1992.	0.8	9

#	Article	IF	Citations
109	Tuning Band Gap Energies in Pb3(C6X6) Extended Solid-State Structures. Journal of Physical Chemistry C, 2012, 116, 8370-8378.	1.5	9
110	The First Molybdenum(VI) and Tungsten(VI) Oxoazides MO₂(N₃)₂, MO₂(N₃)₂â‹…2â€‰CH₃CN, (bipy)MO₂(N₃)₂, and [MO₂(N₃)₄]^{2â^’} (M=Mo, W). Angewandte Chemie - International Edition, 2015, 54, 9581-9585.	7.2	9
111	The niobium oxoazides [NbO(N3)3], [NbO(N3)3Â·2CH3CN], [(bipy)NbO(N3)3], Cs2[NbO(N3)5] and [PPh4]2[NbO(N3)5]. Dalton Transactions, 2016, 45, 10523-10529.	1.6	9
112	Activation of Water by Pentavalent Actinide Dioxide Cations: Characteristic Curium Revealed by a Reactivity Turn after Americium. Inorganic Chemistry, 2019, 58, 14005-14014.	1.9	9
113	Calculated Ionization Potentials of MO₃ and MO₂ for M = U, Mo, W, and Nd. Journal of Physical Chemistry A, 2020, 124, 6913-6919.	1.1	9
114	Effect of initial Î³-irradiation on infrared laser ablation of poly(vinyl alcohol) studied by infrared spectroscopy. Polymer Degradation and Stability, 2020, 181, 109331.	2.7	9
115	Interaction of Th with H^{0/â€“/+}: Combined Experimental and Theoretical Thermodynamic Properties. Journal of Physical Chemistry A, 2022, 126, 198-210.	1.1	9
116	Structural and Theoretical Study of Salts of the [B₉H₁₄]^{â^’} Ion: Isolation of Multiple Isomers and Implications for Energy Storage. ChemPlusChem, 2016, 81, 922-925.	1.3	8
117	1,2-Ethanediol and 1,3-Propanediol Conversions over (MO₃)₃ (M = Mo, W) Nanoclusters: A Computational Study. Journal of Physical Chemistry A, 2016, 120, 1897-1907.	1.1	8
118	Infrared Spectroscopic and Theoretical Studies on the OMF₂ and OMF (M = Cr, Mo, W) Molecules in Solid Argon. Journal of Physical Chemistry A, 2017, 121, 7603-7612.	1.1	8
119	Weakly interacting solvation spheres surrounding a calixarene-protected tetrairidium carbonyl cluster: contrasting effects on reactivity of alkane solvent and silica support. Dalton Transactions, 2018, 47, 13550-13558.	1.6	8
120	Predicting the Formation of Sulfur-Based BrÃ¸nsted Acids from the Reactions of SO_x with H₂O and H₂S. Journal of Physical Chemistry A, 2019, 123, 10169-10183.	1.1	8
121	Synthesis, Structural Characterization, and Coordination Chemistry of (Trineopentylphosphine)palladium(aryl)bromide Dimer Complexes ([(Np₃P)Pd(Ar)Br]₂). Inorganic Chemistry, 2019, 58, 13299-13313.	1.9	8
122	Photodissociation and Theory to Investigate Uranium Oxide Cluster Cations. Journal of Physical Chemistry A, 2020, 124, 1940-1953.	1.1	8
123	Dehydration of UO₂Cl₂Â·3H₂O and Nd(NO₃)₃Â·6H₂O with a Soft Donor Ligand and Comparison of Their Interactions through X-ray Diffraction and Theoretical Investigation. Inorganic Chemistry, 2020, 59, 2861-2869.	1.9	8
124	Th₂O^{â€“}, Th₂Au^{â€“}, and Th₂AuO_{1,2}^{â€“} Anions: Photoelectron Spectroscopic and Computational Characterization of Energetics and Bonding. Journal of Physical Chemistry A, 2021, 125, 258-271.	1.1	8
125	Predicting the Mechanism and Products of CO₂ Capture by Amines in the Presence of H₂O. Journal of Physical Chemistry A, 2021, 125, 9802-9818.	1.1	8
126	Reduction of CO2 to methanol using aluminum ester FLPs. Inorganic Chemistry Communication, 2015, 61, 207-209.	1.8	7

#	Article	IF	Citations
127	In Situ Natural Abundance ¹⁷O and ²⁵Mg NMR Investigation of Aqueous Mg(OH)₂ Dissolution in the Presence of Supercritical CO₂. Environmental Science & Technology, 2016, 50, 12373-12384.	4.6	7
128	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.	1.1	7
129	Role of N-Heterocyclic Carbenes as Ligands in Iridium Carbonyl Clusters. Journal of Physical Chemistry A, 2017, 121, 5029-5044.	1.1	7
130	Preparation and Characterization of Groupâ€…13 Cyanides. Chemistry - A European Journal, 2017, 23, 9054-9066.	1.7	7
131	Hydrolysis of Small Oxo/Hydroxo Molecules Containing High Oxidation State Actinides (Th, Pa, U, Np,) Tj ETQq1 1 0.784314 rgBT /Ov	1.1	7
132	Gas-Phase Acidities of Phosphorylated Amino Acids. Journal of Physical Chemistry B, 2015, 119, 14604-14621.	1.2	6
133	Electronic Structures of Small (RuO₂)_n (n = 1â€“4) Nanoclusters and Their Anions and the Hydrolysis Reactions with Water. Journal of Physical Chemistry A, 2017, 121, 7726-7744.	1.1	6
134	Stability and Electronic Properties of Rocksalt (CdO)_n, (SrO)_n, and (BaO)_n Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 25021-25034.	1.5	6
135	Infrared Spectroscopic and Theoretical Studies of the 3d Transition Metal Oxyfluoride Molecules. Inorganic Chemistry, 2019, 58, 9796-9810.	1.9	6
136	Crystallographic evidence of Watsonâ€“Crick connectivity in the base pair of anionic adenine with thymine. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 18224-18230.	3.3	6
137	Polarizabilities of neutral atoms and atomic ions with a noble gas electron configuration. Journal of Chemical Physics, 2020, 153, 174304.	1.2	6
138	Hydrolysis of Metal Dioxides Differentiates d-block from f-block Elements: Pa(V) as a 6d Transition Metal; Pr(V) as a 4f â€œLanthanylâ€• Journal of Physical Chemistry A, 2020, 124, 9272-9287.	1.1	6
139	Reaction Energetics and ¹³C Fractionation of Alanine Transamination in the Aqueous and Gas Phases. Journal of Physical Chemistry A, 2020, 124, 2077-2089.	1.1	6
140	Prediction of An(III)/Ln(III) Separation by 1,2,4-Triazinylpyridine Derivatives. Journal of Physical Chemistry A, 2021, 125, 6529-6542.	1.1	6
141	Composite Correlated Molecular Orbital Theory Calculations of Ring Strain for Use in Predicting Polymerization Reactions. ChemPhysChem, 2022, , .	1.0	6
142	Die MolybdÃn(V)â€•und Wolfram(VI)â€•oxoazide [MoO(N 3) 3], [MoO(N 3) 3 â‹…2â€‰CH 3 CN], [(bipy)MoO(N 3) 3], [MoO(N 3) 5] 2â¯ , [WO(N 3) 4] und [WO(N 3) 4 â‹…CH 3. Angewandte Chemie, 2015, 127, 15771-15776.	1.6	5
143	Reaction of CO₂ with UO₃ Nanoclusters. Journal of Physical Chemistry A, 2017, 121, 8518-8524.	1.1	5
144	Effect of Radiation from an Infrared Laser and Î³-Rays from 60Co on the Molecularâ€“Topological Structure of Polyvinylidene Fluoride. Journal of Russian Laser Research, 2017, 38, 482-489.	0.3	5

#	Article	IF	Citations
145	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.	1.1	5
146	Pt-Assisted Carbon Remediation of Mo₂C Materials for CO Disproportionation. ACS Catalysis, 2020, 10, 1894-1911.	5.5	5
147	Reaction of NO₂ with Groups IV and VI Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2020, 124, 9222-9236.	1.1	5
148	Thermodynamics of Metal Carbonates and Bicarbonates and Their Hydrates for Mg, Ca, Fe, and Cd Relevant to Mineral Energetics. Journal of Physical Chemistry A, 2020, 124, 1829-1840.	1.1	5
149	Syntheses, solution behavior, and computational bond length analyses of trifluoromethyl and perfluoroethyl cuprate salts. Journal of Fluorine Chemistry, 2020, 234, 109518.	0.9	5
150	Experimental and Computational Description of the Interaction of H and H^{â€“} with U. Journal of Physical Chemistry A, 2022, 126, 4432-4443.	1.1	5
151	NEW CHALLENGES FACING INTEGRATIVE BIOLOGICAL SCIENCE IN THE POST-GENOMIC ERA. Journal of Biological Systems, 2006, 14, 275-293.	0.5	4
152	Active Nanostructures at Interfaces for Photocatalytic Reactors and Low-power Consumption Sensors. Materials Research Society Symposia Proceedings, 2010, 1257, 1.	0.1	4
153	Beyond Relationships Between Homogeneous and Heterogeneous Catalysis. Catalysis Letters, 2014, 144, 1785-1789.	1.4	4
154	The First Molybdenum(VI) and Tungsten(VI) Oxoazides MO 2 (N 3) 2 , MO 2 (N 3) 2 â‹…2â€‰CH 3 CN, (bipy)MO 2 (N 3) 2 , and [MO 2 (N 3) 4] 2â¯ (M=Mo, W). Angewandte Chemie, 2015, 127, 9717-9721.	1.6	4
155	The Binary Groupâ€…4 Azides [PPh₄]₂[Zr(N₃)₆] and [PPh₄]₂[Hf(N₃)₆]. Angewandte Chemie, 2016, 128, 14562-14566.	1.6	4
156	Energetic Properties and Electronic Structure of [Si,N,S] and [Si,P,S] Isomers. Journal of Physical Chemistry A, 2016, 120, 1691-1697.	1.1	4
157	Spectroscopic Characterization of Î¼-Î·¹:Î·¹-Peroxo Ligands Formed by Reaction of Dioxygen with Electron-Rich Iridium Clusters. Inorganic Chemistry, 2019, 58, 14338-14348.	1.9	4
158	Mechanistic Study of Enhanced Protonation by Chromium(III) in Electrospray Ionization: A Superacid Bound to a Peptide. Journal of the American Society for Mass Spectrometry, 2020, 31, 308-318.	1.2	4
159	Impact of Noncovalent Interactions on the Structural Chemistry of Thorium(IV)-Aquo-Chloro Complexes. Inorganic Chemistry, 2021, 60, 6375-6390.	1.9	4
160	Computational Study of Triphosphine-Ligated Cu(I) Catalysts for Hydrogenation of CO₂ to Formate. Journal of Physical Chemistry A, 2021, 125, 6600-6610.	1.1	4
161	Bond Dissociation Energies of Carbeneâ€“Carbene and Carbeneâ€“Main Group Adducts. Journal of Physical Chemistry A, 2022, 126, 2658-2669.	1.1	4
162	Undulating topography of HfO₂ thin films deposited in a mesoscale reactor using hafnium (IV) tert butoxide. AICHE Journal, 2011, 57, 2989-2996.	1.8	3

#	Article	IF	Citations
163	Computational Studies of the NiTi Alloy System: Bulk, Supercell, and Surface Calculations. Materials Research Society Symposia Proceedings, 2011, 1295, 15.	0.1	3
164	Benchmark-Quality Atomization Energies for BeH and BeH₂. Journal of Chemical Theory and Computation, 2017, 13, 649-653.	2.3	3
165	Formation of Cerium and Neodymium Isocyanides in the Reactions of Cyanogen with Ce and Nd Atoms in Argon Matrices. Journal of Physical Chemistry A, 2019, 123, 8208-8219.	1.1	3
166	Experimental and Computational Study of the Gas-Phase Acidities of Acidic Di- and Tripeptides. Journal of Physical Chemistry B, 2019, 123, 606-613.	1.2	3
167	Experimental and Computational Study of the Structure, Steric Properties, and Binding Equilibria of Neopentylphosphine Palladium Complexes. Inorganic Chemistry, 2020, 59, 5579-5592.	1.9	3
168	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	1.2	3
169	Synergistic Coupling of CO₂ and H₂O during Expansion of Clays in Supercritical CO₂â€“CH₄ Fluid Mixtures. Environmental Science & Technology, 2021, 55, 11192-11203.	4.6	3
170	Molecular Properties of Thorium Hydrides: Electron Affinities and Thermochemistry. Journal of Physical Chemistry A, 2022, 126, 2388-2396.	1.1	3
171	Effect of 60Co Î³-radiation on the tetrafluoroethylene/perfluoro(methyl vinyl ether) copolymer. Journal of Fluorine Chemistry, 2020, 240, 109671.	0.9	2
172	Different Carbonate Isomers Formed by the Addition of CO₂ to M₃O₆^{â€“} for M = Ti, Zr, and Hf. Journal of Physical Chemistry A, 2020, 124, 5402-5407.	1.1	2
173	Th(IV) Bromide Complexes: A Homoleptic Aqua Ion and a Novel Th(H₂O)₄Br₄ Structural Unit. Crystal Growth and Design, 2022, 22, 4375-4381.	1.4	2
174	Interfacial Phase Stability in TiV Multilaminate Thin Films. Journal of Physical Chemistry C, 2009, 113, 21383-21388.	1.5	1
175	Preparation and Characterization of Groupâ€…13 Cyanides. Chemistry - A European Journal, 2017, 23, 8991-8991.	1.7	1
176	InnenrÃ¼cktitelbild: Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy (Angew. Chem. 36/2019). Angewandte Chemie, 2019, 131, 12847-12847.	1.6	1
177	Protonation of CH 3 N 3 and CF 3 N 3 in Superacids: Isolation and Structural Characterization of Longâ€Lived Methylâ€and Trifluoromethylamino Diazonium Ions. Angewandte Chemie - International Edition, 2020, 59, 12520-12526.	7.2	1
178	Energetic Properties, Spectroscopy, and Reactivity of NF3O. Journal of Physical Chemistry A, 2020, 124, 5237-5245.	1.1	1
179	A comparison of hydrogen release kinetics from 5- and 6-membered 1,2-BN-cycloalkanes. RSC Advances, 2021, 11, 34132-34136.	1.7	1
180	Electronically Excited Complex Formation in Magnesium Clusterâ€“Halogen Atom Reactions. Journal of Physical Chemistry A, 2022, 126, 1848-1860.	1.1	1

#	Article	IF	Citations
181	Structural and Theoretical Study of Salts of the [B9 H14]â^' Ion: Isolation of Multiple Isomers and Implications for Energy Storage. ChemPlusChem, 2016, 81, 903-903.	1.3	0
182	Energetic Properties and Electronic Structure of [C,N,O,P] and [C,N,S,P] Isomers. Journal of Physical Chemistry A, 2017, 121, 2180-2186.	1.1	0
183	RÃ¼cktitelbild: Formation Mechanism of NF₄⁺ Salts and Extraordinary Enhancement of the Oxidizing Power of Fluorine by Strong Lewis Acids (Angew. Chem. 27/2017). Angewandte Chemie, 2017, 129, 8128-8128.	1.6	0
184	Tungsten Hydride Phosphorus- and Arsenic-Bearing Molecules with Double and Triple Wâ€“P and Wâ€“As Bonds. Inorganic Chemistry, 2018, 57, 5320-5332.	1.9	0
185	Zn_xMg_{60â€“x}O₆₀ Nanoclusters with Tunable Near-Ultraviolet Energy Gaps. Journal of Physical Chemistry C, 2019, 123, 13083-13093.	1.5	0
186	Fluoroâ€nitrogen Cations. Angewandte Chemie, 2022, 134, .	1.6	0
187	Excited Electronic State Cross Sections for Group 3 Halide and Oxide Production: Evaluating Relative Excited-State Quantum Yields. Journal of Physical Chemistry A, 2022, , .	1.1	0
188	Observation of Selectively Populated Monohalide Excited States from the Reactions of Group 3 Metal (Sc, Y, and La) Monomers and Dimers with Halogen-Containing Molecules. Journal of Physical Chemistry A, 0, , .	1.1	0