List of Publications by Year in descending order

267 papers	16,672 citations	17405 63 h-index	17546 121 g-index
272 all docs	272 docs citations	272 times ranked	13928 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.	1.1	9
2	Electronically Excited Complex Formation in Magnesium Clusterâ€“Halogen Atom Reactions. Journal of Physical Chemistry A, 2022, 126, 1848-1860.	1.1	1
3	Bond Dissociation Energies of Carbeneâ€“Carbene and Carbeneâ€“Main Group Adducts. Journal of Physical Chemistry A, 2022, 126, 2658-2669.	1.1	4
4	Molecular Properties of Thorium Hydrides: Electron Affinities and Thermochemistry. Journal of Physical Chemistry A, 2022, 126, 2388-2396.	1.1	3
5	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
6	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
7	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
8	Accelerating the insertion reactions of (NHC)Cuâ€“H via remote ligand functionalization. Chemical Science, 2021, 12, 11495-11505.	3.7	16
9	Solubility thermodynamics of amine boranes in polar solvents. International Journal of Hydrogen Energy, 2021, 46, 10801-10808.	3.8	12
10	Bond Dissociation Energies in Heavy Element Chalcogen and Halogen Small Molecules. Journal of Physical Chemistry A, 2021, 125, 1892-1902.	1.1	10
11	Impact of Noncovalent Interactions on the Structural Chemistry of Thorium(IV)-Aquo-Chloro Complexes. Inorganic Chemistry, 2021, 60, 6375-6390.	1.9	4
12	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	1.2	3
13	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
14	Hydrolysis of Small Oxo/Hydroxo Molecules Containing High Oxidation State Actinides (Th, Pa, U, Np,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.1	7
15	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
16	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
17	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
18	Nature of Oxygen Adsorption on Defective Carbonaceous Materials. Journal of Physical Chemistry C, 2021, 125, 20686-20696.	1.5	11

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19	Investigation of Î³-irradiated polyvinylidene fluoride and its acute toxicity. Journal of Fluorine Chemistry, 2021, 251, 109885.	0.9	2
20	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
21	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
22	Joint influence of Î³â€“irradiation and high temperature shear grinding on the IR spectra and surfaceâ€“energy properties of polyethylene. Polymer, 2021, 237, 124342.	1.8	4
23	A comparison of hydrogen release kinetics from 5- and 6-membered 1,2-BN-cycloalkanes. RSC Advances, 2021, 11, 34132-34136.	1.7	1
24	Pt-Assisted Carbon Remediation of Mo₂C Materials for CO Disproportionation. ACS Catalysis, 2020, 10, 1894-1911.	5.5	5
25	Reaction of NO₂ with Groups IV and VI Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2020, 124, 9222-9236.	1.1	5
26	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
27	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
28	Polarizabilities of neutral atoms and atomic ions with a noble gas electron configuration. Journal of Chemical Physics, 2020, 153, 174304.	1.2	6
29	Effect of 60Co Î³-radiation on the tetrafluoroethylene/perfluoro(methyl vinyl ether) copolymer. Journal of Fluorine Chemistry, 2020, 240, 109671.	0.9	2
30	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
31	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
32	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
33	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
34	Energetic Properties, Spectroscopy, and Reactivity of NF3O. Journal of Physical Chemistry A, 2020, 124, 5237-5245.	1.1	1
35	Lewis Acidity and Basicity: Another Measure of Carbene Reactivity. Journal of Physical Chemistry A, 2020, 124, 6096-6103.	1.1	11
36	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

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37	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
38	Mechanism of selective and complete oxidation in La₂O₃-catalyzed oxidative coupling of methane. Catalysis Science and Technology, 2020, 10, 2602-2614.	2.1	28
39	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
40	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
41	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
42	Direct fluorination of tetrafluoroethylene at low temperatures. Journal of Fluorine Chemistry, 2020, 232, 109493.	0.9	3
43	Photodissociation and Theory to Investigate Uranium Oxide Cluster Cations. Journal of Physical Chemistry A, 2020, 124, 1940-1953.	1.1	8
44	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
45	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
46	Syntheses, solution behavior, and computational bond length analyses of trifluoromethyl and perfluoroethyl cuprate salts. Journal of Fluorine Chemistry, 2020, 234, 109518.	0.9	5
47	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
48	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
49	Predictive Acid Gas Adsorption in Rare Earth DOBDC Metalâ€“Organic Frameworks via Complementary Cluster and Periodic Structure Models. Journal of Physical Chemistry C, 2020, 124, 26801-26813.	1.5	25
50	Infrared Spectroscopic and Theoretical Studies of the 3d Transition Metal Oxyfluoride Molecules. Inorganic Chemistry, 2019, 58, 9796-9810.	1.9	6
51	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
52	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
53	Effect of X-ray beam on the molecularâ€“topological structure of the surface of kynarÂ® polyvinylidene fluoride resin. Journal of Fluorine Chemistry, 2019, 226, 109338.	0.9	5
54	Monomeric and Trimeric Thorium Chlorides Isolated from Acidic Aqueous Solution. Inorganic Chemistry, 2019, 58, 10871-10882.	1.9	12

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55	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
56	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
57	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
58	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
59	MgO-Supported Iridium Metal Pair-Site Catalysts Are More Active and Resistant to CO Poisoning than Analogous Single-Site Catalysts for Ethylene Hydrogenation and Hydrogenâ€“Deuterium Exchange. ACS Catalysis, 2019, 9, 9545-9553.	5.5	25
60	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
61	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
62	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
63	Understanding the Binding of Aromatic Hydrocarbons on Rutile TiO₂(110). Journal of Physical Chemistry C, 2019, 123, 16766-16777.	1.5	16
64	Surface-Catalyzed Oxygen Exchange during Mineral Carbonation in Nanoscale Water Films. Journal of Physical Chemistry C, 2019, 123, 12871-12885.	1.5	21
65	Zn_xMg_{60â€“x}O₆₀ Nanoclusters with Tunable Near-Ultraviolet Energy Gaps. Journal of Physical Chemistry C, 2019, 123, 13083-13093.	1.5	0
66	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
67	Raman Spectroscopy Investigation of Polytetrafluoroethylene in Different Zones of Impact of Continuous CO2 Laser Radiation. Journal of Russian Laser Research, 2019, 40, 571-580.	0.3	0
68	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
69	Electronic Structure Predictions of the Energetic Properties of Tellurium Fluorides. Inorganic Chemistry, 2019, 58, 8279-8292.	1.9	10
70	Energetics of CO2â€“ in Aqueous Solution. Journal of Physical Chemistry A, 2019, 123, 1243-1259.	1.1	11
71	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
72	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

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73	Chemistry of the Highly Strained Alkene Perfluorobicyclo[2.2.0]hexâ€1(4)â€ene. European Journal of Organic Chemistry, 2018, 2018, 3167-3179.	1.2	2
74	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
75	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
76	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
77	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
78	Beating Heterogeneity of Single-Site Catalysts: MgO-Supported Iridium Complexes. ACS Catalysis, 2018, 8, 3489-3498.	5.5	64
79	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
80	Boranes with Ultra-High Stokes Shift Fluorescence. Organometallics, 2018, 37, 3732-3741.	1.1	40
81	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
82	Î±â€Fluoroalcohols: Synthesis and Characterization of Perfluorinated Methanol, Ethanol and nâ€Propanol, and their Oxonium Salts. Chemistry - A European Journal, 2018, 24, 16737-16742.	1.7	5
83	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
84	Water Structure Controls Carbonic Acid Formation in Adsorbed Water Films. Journal of Physical Chemistry Letters, 2018, 9, 4988-4994.	2.1	16
85	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
86	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
87	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
88	Benchmark-Quality Atomization Energies for BeH and BeH₂. Journal of Chemical Theory and Computation, 2017, 13, 649-653.	2.3	3
89	Acid Gas Adsorption on Metalâ€“Organic Framework Nanosheets as a Model of an â€œAll-Surfaceâ€• Material. Journal of Chemical Theory and Computation, 2017, 13, 1341-1350.	2.3	23
90	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

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91	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
92	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
93	Formation and Characterization of Homoleptic Thorium Isocyanide Complexes. Inorganic Chemistry, 2017, 56, 5060-5068.	1.9	20
94	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
95	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
96	Modeling the formation of TiO₂ ultra-small nanoparticles. Nanoscale, 2017, 9, 7143-7162.	2.8	21
97	Role of N-Heterocyclic Carbenes as Ligands in Iridium Carbonyl Clusters. Journal of Physical Chemistry A, 2017, 121, 5029-5044.	1.1	7
98	Highâ€Energyâ€Resolution Xâ€ray Absorption Spectroscopy for Identification of Reactive Surface Species on Supported Singleâ€Site Iridium Catalysts. Chemistry - A European Journal, 2017, 23, 14760-14768.	1.7	35
99	Singleâ€Site Osmium Catalysts on MgO: Reactivity and Catalysis of CO Oxidation. Chemistry - A European Journal, 2017, 23, 2532-2536.	1.7	18
100	Reaction of CO₂ with UO₃ Nanoclusters. Journal of Physical Chemistry A, 2017, 121, 8518-8524.	1.1	5
101	Reaction of CO₂ with Groups 4 and 6 Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2017, 121, 8719-8727.	1.1	13
102	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
103	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
104	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
105	Structures and Stabilities of (CaO)_n Nanoclusters. Journal of Physical Chemistry C, 2017, 121, 23025-23038.	1.5	14
106	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO₂. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791.	4.0	38
107	Reaction of SO2 with Group IV and VI transition metal oxide clusters. Computational and Theoretical Chemistry, 2017, 1120, 46-55.	1.1	6
108	Atomically dispersed supported metal catalysts: perspectives and suggestions for future research. Catalysis Science and Technology, 2017, 7, 4259-4275.	2.1	221

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109	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
110	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
111	Uranium(IV) Chloride Complexes: UCl₆^{2â€“} and an Unprecedented U(H₂O)₄Cl₄ Structural Unit. Inorganic Chemistry, 2017, 56, 9772-9780.	1.9	21
112	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
113	A Modular Synthetic Approach to Monocyclic 1,4â€Azaborines. Angewandte Chemie - International Edition, 2016, 55, 8333-8337.	7.2	50
114	The Synthesis, Characterization and Dehydrogenation of Sigmaâ€Complexes of BNâ€Cyclohexanes. Chemistry - A European Journal, 2016, 22, 310-322.	1.7	22
115	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
116	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
117	Substituent Effects on the Properties of Borafluorenes. Organometallics, 2016, 35, 3182-3191.	1.1	58
118	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
119	Synthesis of nanoscale silicon oxide oxidation state distributions: The transformation from hydrophilicity to hydrophobicity. Chemical Physics Letters, 2016, 653, 137-143.	1.2	5
120	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
121	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
122	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
123	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie - International Edition, 2015, 54, 7823-7827.	7.2	49
124	Singleâ€Site Zeoliteâ€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
125	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie, 2015, 127, 7934-7938.	1.6	17
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127	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
128	Structures, relative energies, and ligand dissociation energies of iridium carbonyl phosphine clusters. Computational and Theoretical Chemistry, 2015, 1069, 18-35.	1.1	2
129	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
130	Structures and Energetics of (MgCO₃)_n Clusters (n â‰¤ 16). Journal of Physical Chemistry A, 2015, 119, 3419-3428.	1.1	18
131	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
132	Prediction of the pK_aâ€™s of Aqueous Metal Ion +2 Complexes. Journal of Physical Chemistry A, 2015, 119, 2926-2939.	1.1	67
133	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
134	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
135	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
136	Reactions of laser-ablated U atoms with (CN)2: infrared spectra and electronic structure calculations of UNC, U(NC)2, and U(NC)4 in solid argon. Chemical Communications, 2015, 51, 3899-3902.	2.2	26
137	Molecular models of site-isolated cobalt, rhodium, and iridium catalysts supported on zeolites: Ligand bond dissociation energies. Computational and Theoretical Chemistry, 2015, 1074, 58-72.	1.1	14
138	Gas-Phase Acidities of Phosphorylated Amino Acids. Journal of Physical Chemistry B, 2015, 119, 14604-14621.	1.2	6
139	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
140	Bis-BN Cyclohexane: A Remarkably Kinetically Stable Chemical Hydrogen Storage Material. Journal of the American Chemical Society, 2015, 137, 134-137.	6.6	62
141	Selective molecular recognition by nanoscale environments in a supported iridium cluster catalyst. Nature Nanotechnology, 2014, 9, 459-465.	15.6	53
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