Monica Vasiliu

List of Publications by Year
in descending order

96 papers	1,995 citations	257450 24 h-index	289244 40 g-index
102 all docs	102 docs citations	102 times ranked	2454 citing authors

#	Article	IF	Citations
1	Emergence of californium as the second transitional element in the actinide series. Nature Communications, 2015, 6, 6827.	12.8	108
2	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.	13.7	100
3	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_{<i>X</i>} Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 12609-12616.	13.8	96
4	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
5	Electrochemical Conversion of Muconic Acid to Biobased Diacid Monomers. ACS Sustainable Chemistry and Engineering, 2016, 4, 3575-3585.	6.7	81
6	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.	13.7	80
7	BN-substituted diphenylacetylene: a basic model for conjugated Ï€-systems containing the BN bond pair. Chemical Science, 2012, 3, 825-829.	7.4	66
8	Perfluoroalkyl Cobalt(III) Fluoride and Bis(perfluoroalkyl) Complexes: Catalytic Fluorination and Selective Difluorocarbene Formation. Journal of the American Chemical Society, 2015, 137, 16064-16073.	13.7	63
9	Substituent Effects on the Properties of Borafluorenes. Organometallics, 2016, 35, 3182-3191.	2.3	58
10	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
11	Investigation of the Structure and Active Sites of TiO₂ Nanorod Supported VO_{<i>x</i>} Catalysts by High-Field and Fast-Spinning ⁵¹V MAS NMR. ACS Catalysis, 2015, 5, 3945-3952.	11.2	51
12	A Modular Synthetic Approach to Monocyclic 1,4â€Azaborines. Angewandte Chemie - International Edition, 2016, 55, 8333-8337.	13.8	50
13	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie - International Edition, 2015, 54, 7823-7827.	13.8	49
14	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_{<i>X</i>} Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie, 2019, 131, 12739-12746.	2.0	45
15	Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds: Fluorides, Chlorides, Oxides, and Hydroxides for Be, Mg, and Ca. Journal of Physical Chemistry A, 2010, 114, 9349-9358.	2.5	43
16	Spectroscopic and Energetic Properties of Thorium(IV) Molecular Clusters with a Hexanuclear Core. Journal of Physical Chemistry A, 2012, 116, 6917-6926.	2.5	43
17	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
18	Boranes with Ultra-High Stokes Shift Fluorescence. Organometallics, 2018, 37, 3732-3741.	2.3	40

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19	Investigation of Silica-Supported Vanadium Oxide Catalysts by High-Field ⁵¹V Magic-Angle Spinning NMR. Journal of Physical Chemistry C, 2017, 121, 6246-6254.	3.1	39
20	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
21	Electrochemical and Spectroscopic Properties of Boron Dipyrrometheneâ€“Thiopheneâ€“Triphenylamine-Based Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2016, 120, 9068-9080.	3.1	36
22	Are DTTO and <i>iso</i>â€DTTO Worthwhile Targets for Synthesis?. Propellants, Explosives, Pyrotechnics, 2015, 40, 463-468.	1.6	34
23	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.	11.2	31
24	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.	3.1	30
25	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.	11.2	25
26	Initial Steps in the Selective Catalytic Reduction of NO with NH₃ by TiO₂-Supported Vanadium Oxides. ACS Catalysis, 2020, 10, 13918-13931.	11.2	22
27	Uranium(IV) Chloride Complexes: UCl₆^{2â€“} and an Unprecedented U(H₂O)₄Cl₄ Structural Unit. Inorganic Chemistry, 2017, 56, 9772-9780.	4.0	21
28	A Modular Synthetic Approach to Monocyclic 1,4â€Azaborines. Angewandte Chemie, 2016, 128, 8473-8477.	2.0	20
29	F⁺ and F^{âˆ’} Affinities of Simple N_{<i>x</i>}F_{<i>y</i>} and O_{<i>x</i>}F_{<i>y</i>} Compounds. Inorganic Chemistry, 2011, 50, 1914-1925.	4.0	19
30	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
31	How Energetic are <i>cyclo</i>â€Pentazolates?. Propellants, Explosives, Pyrotechnics, 2019, 44, 263-266.	1.6	19
32	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
33	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie, 2015, 127, 7934-7938.	2.0	17
34	Metal Heptafluoroisopropyl (M-hfip) Complexes for Use as hfip Transfer Agents. Organometallics, 2018, 37, 422-432.	2.3	17
35	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
36	Water Structure Controls Carbonic Acid Formation in Adsorbed Water Films. Journal of Physical Chemistry Letters, 2018, 9, 4988-4994.	4.6	16

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37	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
38	Accelerating the insertion reactions of (NHC)Cuâ€"H <i>via</i> remote ligand functionalization. Chemical Science, 2021, 12, 11495-11505.	7.4	16
39	Heats of Formation of MH_{<i>x</i>}Cl_{<i>y</i>} (M = Si, P, As, Sb) Compounds and Main Group Fluorides from High Level Electronic Structure Calculations. Journal of Physical Chemistry A, 2012, 116, 3717-3727.	2.5	14
40	The Vanadium(V) Oxoazides [VO(N₃)₃], [(bipy)VO(N₃)₃], and [VO(N₃)₅]^{2â^’}. Angewandte Chemie - International Edition, 2015, 54, 9101-9105.	13.8	14
41	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.	3.3	14
42	Synthesis of 1<i>H</i>-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.	3.2	14
43	Prediction of the Thermodynamic Properties of Key Products and Intermediates from Biomass. II. Journal of Physical Chemistry C, 2012, 116, 20738-20754.	3.1	13
44	Preparation and Characterization of Antimony and Arsenic Tricyanide and Their 2,2â€²â€Bipyridine Adducts. Chemistry - A European Journal, 2016, 22, 13251-13257.	3.3	12
45	Monomeric and Trimeric Thorium Chlorides Isolated from Acidic Aqueous Solution. Inorganic Chemistry, 2019, 58, 10871-10882.	4.0	12
46	The Binary Groupâ€…4 Azides [PPh₄]₂[Zr(N₃)₆] and [PPh₄]₂[Hf(N₃)₆]. Angewandte Chemie - International Edition, 2016, 55, 14350-14354.	13.8	11
47	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
48	Lewis Acidity and Basicity: Another Measure of Carbene Reactivity. Journal of Physical Chemistry A, 2020, 124, 6096-6103.	2.5	11
49	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.	13.8	10
50	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.	2.5	10
51	Electronic Structure Predictions of the Energetic Properties of Tellurium Fluorides. Inorganic Chemistry, 2019, 58, 8279-8292.	4.0	10
52	Bond Dissociation Energies in Heavy Element Chalcogen and Halogen Small Molecules. Journal of Physical Chemistry A, 2021, 125, 1892-1902.	2.5	10
53	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.	3.3	9
54	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

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55	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
56	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
57	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.	2.5	8
58	Synthesis, Structural Characterization, and Coordination Chemistry of (Trineopentylphosphine)palladium(aryl)bromide Dimer Complexes ([(Np₃P)Pd(Ar)Br]₂). Inorganic Chemistry, 2019, 58, 13299-13313.	4.0	8
59	Photodissociation and Theory to Investigate Uranium Oxide Cluster Cations. Journal of Physical Chemistry A, 2020, 124, 1940-1953.	2.5	8
60	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.	4.0	8
61	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.	2.5	8
62	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
63	Preparation and Characterization of Groupâ€…13 Cyanides. Chemistry - A European Journal, 2017, 23, 9054-9066.	3.3	7
64	Hydrolysis of Small Oxo/Hydroxo Molecules Containing High Oxidation State Actinides (Th, Pa, U, Np,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.5	7
65	Stability and Electronic Properties of Rocksalt (CdO)_{<i>n</i>}, (SrO)_{<i>n</i>}, and (BaO)_{<i>n</i>} Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 25021-25034.	3.1	6
66	Infrared Spectroscopic and Theoretical Studies of the 3d Transition Metal Oxyfluoride Molecules. Inorganic Chemistry, 2019, 58, 9796-9810.	4.0	6
67	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.	2.5	6
68	Prediction of An(III)/Ln(III) Separation by 1,2,4-Triazinylpyridine Derivatives. Journal of Physical Chemistry A, 2021, 125, 6529-6542.	2.5	6
69	Computational Study of Molecular Hydrogen Adsorption over Small (MO₂)_{<i>n</i>} Nanoclusters (M = Ti, Zr, Hf; <i>n</i> = 1 to 4). Journal of Physical Chemistry A, 2018, 122, 4338-4349.	2.5	5
70	Î±â€Fluoroalcohols: Synthesis and Characterization of Perfluorinated Methanol, Ethanol and <i>n</i>â€Propanol, and their Oxonium Salts. Chemistry - A European Journal, 2018, 24, 16737-16742.	3.3	5
71	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.	2.5	5
72	Experimental and Computational Description of the Interaction of H and H^{â€“} with U. Journal of Physical Chemistry A, 2022, 126, 4432-4443.	2.5	5

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73	The Binary Groupâ€…4 Azides [PPh₄]₂[Zr(N₃)₆] and [PPh₄]₂[Hf(N₃)₆]. Angewandte Chemie, 2016, 128, 14562-14566.	2.0	4
74	Impact of Noncovalent Interactions on the Structural Chemistry of Thorium(IV)-Aquo-Chloro Complexes. Inorganic Chemistry, 2021, 60, 6375-6390.	4.0	4
75	Bond Dissociation Energies of Carbeneâ€"Carbene and Carbeneâ€"Main Group Adducts. Journal of Physical Chemistry A, 2022, 126, 2658-2669.	2.5	4
76	Benchmark-Quality Atomization Energies for BeH and BeH₂. Journal of Chemical Theory and Computation, 2017, 13, 649-653.	5.3	3
77	Formation Mechanism of NF 4 + Salts and Extraordinary Enhancement of the Oxidizing Power of Fluorine by Strong Lewis Acids. Angewandte Chemie, 2017, 129, 8032-8037.	2.0	3
78	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.	2.5	3
79	Experimental and Computational Study of the Structure, Steric Properties, and Binding Equilibria of Neopentylphosphine Palladium Complexes. Inorganic Chemistry, 2020, 59, 5579-5592.	4.0	3
80	Synergistic Coupling of CO₂ and H₂O during Expansion of Clays in Supercritical CO₂â€"CH₄ Fluid Mixtures. Environmental Science & Technology, 2021, 55, 11192-11203.	10.0	3
81	Molecular Properties of Thorium Hydrides: Electron Affinities and Thermochemistry. Journal of Physical Chemistry A, 2022, 126, 2388-2396.	2.5	3
82	Chemistry of the Highly Strained Alkene Perfluorobicyclo[2.2.0]hexâ€•1(4)â€•ene. European Journal of Organic Chemistry, 2018, 2018, 3167-3179.	2.4	2
83	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.	2.5	2
84	Th(IV) Bromide Complexes: A Homoleptic Aqua Ion and a Novel Th(H₂O)₄Br₄ Structural Unit. Crystal Growth and Design, 2022, 22, 4375-4381.	3.0	2
85	Preparation and Characterization of Groupâ€…13 Cyanides. Chemistry - A European Journal, 2017, 23, 8991-8991.	3.3	1
86	InnenrÃ¼cktitelbild: Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_{<i>X</i>} Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy (Angew. Chem. 36/2019). Angewandte Chemie, 2019, 131, 12847-12847.	2.0	1
87	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.	13.8	1
88	Energetic Properties, Spectroscopy, and Reactivity of NF3O. Journal of Physical Chemistry A, 2020, 124, 5237-5245.	2.5	1
89	A comparison of hydrogen release kinetics from 5- and 6-membered 1,2-BN-cycloalkanes. RSC Advances, 2021, 11, 34132-34136.	3.6	1
90	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.	2.0	0

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91	Tungsten Hydride Phosphorus- and Arsenic-Bearing Molecules with Double and Triple Wâ€“P and Wâ€“As Bonds. Inorganic Chemistry, 2018, 57, 5320-5332.	4.0	0
92	Î±â€Fluoroalcohols: Synthesis and Characterization of Perfluorinated Methanol, Ethanol and n â€Propanol, and their Oxonium Salts. Chemistry - A European Journal, 2018, 24, 16701-16701.	3.3	0
93	Frontispiece: Gas Phase Hydrolysis and Oxoâ€Exchange of Actinide Dioxide Cations: Elucidating Intrinsic Chemistry from Protactinium to Einsteinium. Chemistry - A European Journal, 2019, 25, .	3.3	0
94	Raman Spectroscopy Investigation of Polytetrafluoroethylene in Different Zones of Impact of Continuous CO2 Laser Radiation. Journal of Russian Laser Research, 2019, 40, 571-580.	0.6	0
95	Protonierung von CH 3 N 3 und CF 3 N 3 in SupersÃuren: Isolierung und strukturelle Charakterisierung von langlebigen Methylâ€•und Trifluormethylaminoâ€Diazoniumâ€Ionen. Angewandte Chemie, 2020, 132, 12620-12627.	2.0	0
96	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, , .	2.5	0