Shiv N Khanna

List of Publications by Year
in descending order

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#	Article	IF	Citations
1	Cluster-Assembled Materials. ACS Nano, 2009, 3, 244-255.	14.6	598
2	Formation of Al13I-: Evidence for the Superhalogen Character of Al13. Science, 2004, 304, 84-87.	12.6	515
3	Reactivity of Metal Clusters. Chemical Reviews, 2016, 116, 14456-14492.	47.7	359
4	Complementary Active Sites Cause Size-Selective Reactivity of Aluminum Cluster Anions with Water. Science, 2009, 323, 492-495.	12.6	262
5	Designer magnetic superatoms. Nature Chemistry, 2009, 1, 310-315.	13.6	223
6	Preparation of Elemental Cu and Ni Nanoparticles by the Polyol Method: An Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2011, 115, 2656-2664.	3.1	217
7	Superatoms: Electronic and Geometric Effects on Reactivity. Accounts of Chemical Research, 2017, 50, 255-263.	15.6	203
8	A Systematic Framework and Nanoperiodic Concept for Unifying Nanoscience: Hard/Soft Nanoelements, Superatoms, Meta-Atoms, New Emerging Properties, Periodic Property Patterns, and Predictive Mendeleev-like Nanoperiodic Tables. Chemical Reviews, 2016, 116, 2705-2774.	47.7	195
9	Superatom Compounds, Clusters, and Assemblies:â€‰ Ultra Alkali Motifs and Architectures. Journal of the American Chemical Society, 2007, 129, 10189-10194.	13.7	186
10	Spin Accommodation and Reactivity of Aluminum Based Clusters with O₂. Journal of the American Chemical Society, 2007, 129, 16098-16101.	13.7	147
11	Cluster-Assembled Materials: Toward Nanomaterials with Precise Control over Properties. ACS Nano, 2010, 4, 235-240.	14.6	127
12	Spin Accommodation and Reactivity of Silver Clusters with Oxygen: The Enhanced Stability of Ag₁₃^{â€“}. Journal of the American Chemical Society, 2012, 134, 18973-18978.	13.7	114
13	From Designer Clusters to Synthetic Crystalline Nanoassemblies. Nano Letters, 2007, 7, 2734-2741.	9.1	109
14	On the Existence of Designer Magnetic Superatoms. Journal of the American Chemical Society, 2013, 135, 4856-4861.	13.7	108
15	Hundâ€™s rule in superatoms with transition metal impurities. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10062-10066.	7.1	105
16	Reactivity of Aluminum Cluster Anions with Water: Origins of Reactivity and Mechanisms for H₂ Release. Journal of Physical Chemistry A, 2010, 114, 6071-6081.	2.5	95
17	Probing the Magic Numbers of Aluminumâ€“Magnesium Cluster Anions and Their Reactivity toward Oxygen. Journal of the American Chemical Society, 2013, 135, 4307-4313.	13.7	88
18	Controlling the Band Gap Energy of Cluster-Assembled Materials. Accounts of Chemical Research, 2013, 46, 2385-2395.	15.6	81

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19	On the Ground State of Pd₁₃. Journal of the American Chemical Society, 2011, 133, 12192-12196.	13.7	74
20	Controlling Band Gap Energies in Cluster-Assembled Ionic Solids through Internal Electric Fields. ACS Nano, 2010, 4, 5813-5818.	14.6	72
21	What determines if a ligand activates or passivates a superatom cluster?. Chemical Science, 2016, 7, 3067-3074.	7.4	67
22	Magnetic properties of Co2C and Co3C nanoparticles and their assemblies. Applied Physics Letters, 2012, 101, .	3.3	64
23	Crystal field effects on the reactivity of aluminum-copper cluster anions. Physical Review B, 2010, 81, .	3.2	59
24	Does the 18-Electron Rule Apply to CrSi₁₂?. Journal of Physical Chemistry Letters, 2014, 5, 3492-3496.	4.6	56
25	Nature of Valence Transition and Spin Moment in Ag_{<i>n</i>}V⁺ Clusters. Journal of the American Chemical Society, 2014, 136, 8229-8236.	13.7	53
26	Synthesis and Structural Characterization of an Atom-Precise Bimetallic Nanocluster, Ag₄Ni₂(DMSA)₄. Journal of the American Chemical Society, 2013, 135, 26-29.	13.7	51
27	Metal Chalcogenide Clusters with Closed Electronic Shells and the Electronic Properties of Alkalis and Halogens. Journal of the American Chemical Society, 2017, 139, 1871-1877.	13.7	51
28	Reactions of AlnIx-with Methyl Iodide:â€‰ The Enhanced Stability of Al7I and the Chemical Significance of Active Centers. Journal of the American Chemical Society, 2005, 127, 16048-16053.	13.7	46
29	Ligand-Induced Active Sites: Reactivity of Iodine-Protected Aluminum Superatoms with Methanol. Journal of the American Chemical Society, 2012, 134, 20507-20512.	13.7	46
30	From SiO Molecules to Silicates in Circumstellar Space: Atomic Structures, Growth Patterns, and Optical Signatures of Si_{<i>n</i>}O_{<i>m</i>} Clusters. ACS Nano, 2008, 2, 1729-1737.	14.6	45
31	Ni₉Te₆(PEt₃)₈C₆₀ Is a Superatomic Superalkali Superparamagnetic Cluster Assembled Material (S³-CAM). Journal of the American Chemical Society, 2016, 138, 1916-1921.	13.7	42
32	Edge-Induced Active Sites Enhance the Reactivity of Large Aluminum Cluster Anions with Alcohols. Journal of Physical Chemistry A, 2012, 116, 8085-8091.	2.5	41
33	Electronic subshell splitting controls the atomic structure of charged and neutral silver clusters. New Journal of Chemistry, 2013, 37, 3928.	2.8	36
34	Strong lowering of ionization energy of metallic clusters by organic ligands without changing shell filling. Nature Communications, 2018, 9, 2357.	12.8	34
35	Synthesis, structure and band gap energy of covalently linked cluster-assembled materials. Dalton Transactions, 2012, 41, 12365.	3.3	33
36	Evolution of the Spin Magnetic Moments and Atomic Valence of Vanadium in VCu_{<i>x</i>}⁺, VAg_{<i>x</i>}⁺, and VAu_{<i>x</i>}⁺ Clusters (<i>x</i> = 3â€“14). Journal of Physical Chemistry A, 2017, 121, 2990-2999.	2.5	31

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37	Al_{<i>n</i>}Bi Clusters: Transitions Between Aromatic and Jellium Stability. Journal of Physical Chemistry A, 2008, 112, 13316-13325.	2.5	29
38	Shell magnetism in transition metal doped calcium superatom. Chemical Physics Letters, 2012, 528, 39-43.	2.6	28
39	Highly efficient (Cs8V) superatom-based spin-polarizer. Applied Physics Letters, 2009, 95, .	3.3	26
40	Effect of Electronic and Geometric Shell Closures on the Stability of Neutral and Anionic TiNa_{<i>n</i>} (<i>n</i> = 1âˆ’13) Clusters. Journal of Physical Chemistry C, 2010, 114, 10739-10744.	3.1	26
41	Boron Substitution in Aluminum Cluster Anions: Magic Clusters and Reactivity with Oxygen. Journal of Physical Chemistry A, 2014, 118, 8485-8492.	2.5	24
42	Tuning the electronic properties of hexanuclear cobalt sulfide superatoms <i>via</i> ligand substitution. Chemical Science, 2019, 10, 1760-1766.	7.4	24
43	Combined Experimental and Theoretical Study of Al_{<i>n</i>}X (<i>n</i>= 1âˆ’6; X = As, Sb) Clusters: Evidence of Aromaticity and the Jellium Model. Journal of Physical Chemistry A, 2010, 114, 2045-2052.	2.5	23
44	Effect of Charge and Composition on the Structural Fluxionality and Stability of Nine Atom Tinâˆ’Bismuth Zintl Analogues. Inorganic Chemistry, 2008, 47, 10953-10958.	4.0	22
45	Geometry controls the stability of FeSi₁₄. Physical Chemistry Chemical Physics, 2015, 17, 15718-15724.	2.8	21
46	Transforming Ni₉Te₆ from Electron Donor to Acceptor via Ligand Exchange. Journal of Physical Chemistry A, 2016, 120, 6644-6649.	2.5	20
47	The Zintl ion [As7]2âˆ’: an example of an electron-deficient Asx radical anion. Chemical Communications, 2011, 47, 3126.	4.1	18
48	Cooperative effects in the oxidation of CO by palladium oxide cations. Journal of Chemical Physics, 2011, 135, 234303.	3.0	18
49	The applicability of three-dimensional aromaticity in BiSnnâˆ’ Zintl analogues. Journal of Chemical Physics, 2010, 133, 134302.	3.0	17
50	Magnetism of electrons in atoms and superatoms. Journal of Applied Physics, 2012, 112, 064313.	2.5	17
51	IN QUEST OF A SYSTEMATIC FRAMEWORK FOR UNIFYING AND DEFINING NANOSCIENCE. Modern Physics Letters B, 2014, 28, 1430002.	1.9	17
52	Electronic structure, stability, and oxidation of boron-magnesium clusters and cluster solids. Journal of Chemical Physics, 2015, 142, 054304.	3.0	17
53	Ionic versus metallic bonding in AlnNam and AlnMgm (m â‰ 3, n + m â‰ 15) clusters. Journal of Chemical Physics, 2017, 146, 224301.	3.0	17
54	Robust Magnetic Moments on Impurities in Metallic Clusters: Localized Magnetic States in Superatoms. Journal of Physical Chemistry A, 2013, 117, 4297-4303.	2.5	16

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55	Anion Photoelectron Spectroscopy and First-Principles Study of Pb_{<i>x</i>}In_{<i>y</i>} Clusters. Journal of Physical Chemistry C, 2010, 114, 20907-20916.	3.1	15
56	Superatomic molecules with internal electric fields for light harvesting. Nanoscale, 2020, 12, 4736-4742.	5.6	15
57	Metallic and molecular orbital concepts in XMg8 clusters, X = Be-F. Journal of Chemical Physics, 2012, 136, 134311.	3.0	14
58	Resilient aromaticity in leadâ€“indium clusters. Chemical Physics Letters, 2010, 500, 196-201.	2.6	13
59	Making sense of the conflicting magic numbers in WSin clusters. Journal of Chemical Physics, 2015, 143, 074310.	3.0	13
60	Preparation of gas phase naked silver cluster cations outside a mass spectrometer from ligand protected clusters in solution. Nanoscale, 2018, 10, 15714-15722.	5.6	13
61	Ligand Effect on the Electronic Structure of Cobalt Sulfide Clusters: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 25121-25127.	3.1	13
62	The Oblate Structure and Unexpected Resistance in Reactivity of Ag₁₅⁺ with O₂. Journal of Physics: Conference Series, 2013, 438, 012002.	0.4	12
63	Reactivity of Silver Clusters Anions with Ethanethiol. Journal of Physical Chemistry A, 2014, 118, 8345-8350.	2.5	12
64	Atom precise platinumâ€“thiol crowns. Nanoscale, 2015, 7, 19448-19452.	5.6	12
65	Strong Effect of Organic Ligands on the Electronic Structure of Metal-Chalcogenide Clusters. Journal of Physical Chemistry A, 2018, 122, 6014-6020.	2.5	12
66	Helical and linear [K(As11)]2âˆ' chains: Role of solvent on the conformation of chains formed by Zintl anions. Chemical Physics Letters, 2009, 473, 305-311.	2.6	11
67	CO ligands stabilize metal chalcogenide Co₆Se₈(CO)_n clusters <i>via</i> demagnetization. Physical Chemistry Chemical Physics, 2017, 19, 31940-31948.	2.8	11
68	Electronic and magnetic properties of Fe2Sin (1â€¯â‰¤â€¯nâ€¯â‰¤â€¯12)+/0/âˆ' clusters. Chemical Physics Letters, 2018, 706, 113-119.	2.6	11
69	Complete Ag₄M₂(DMSA)₄ (M = Ni, Pd, Pt, DMSA =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5 Characterization. Journal of Physical Chemistry A, 2017, 121, 5324-5331.	2.5	10
70	One-Dimensional Silver-Thiolate Cluster-Assembly: Effect of Argentophilic Interactions on Excited-State Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 2154-2159.	4.6	10
71	Palladium in the Gap: Cluster Assemblies with Band Edges Localized on Linkers. Journal of Physical Chemistry C, 2012, 116, 10207-10214.	3.1	9
72	Effect of Embedding Platinum Clusters in Alumina on Sintering, Coking, and Activity. Journal of Physical Chemistry C, 2017, 121, 21527-21534.	3.1	9

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73	Metal Clusters and Their Reactivity. , 2020, , .		9
74	The superatomic state beyond conventional magic numbers: Ligated metal chalcogenide superatoms. Journal of Chemical Physics, 2021, 155, 120901.	3.0	9
75	Stability and electronic properties of isoelectronic heteroatomic analogs of. Chemical Physics Letters, 2011, 505, 92-95.	2.6	8
76	The Effects of Alkaline-Earth Counterions on the Architectures, Band-Gap Energies, and Proton Transfer of Triazole-Based Coordination Polymers. European Journal of Inorganic Chemistry, 2015, 2015, 2085-2091.	2.0	8
77	High-Spin Superatom Stabilized by Dual Subshell Filling. Journal of the American Chemical Society, 2022, 144, 5172-5179.	13.7	8
78	Closed-shell to split-shell stability of isovalent clusters. Physical Review B, 2011, 84, .	3.2	7
79	Magnetic properties of Co2â^’xTMxC and Co3â^’xTMxC nanoparticles. Journal of Applied Physics, 2013, 114, 243909.	2.5	7
80	Al Valence Controls the Coordination and Stability of Cationic Aluminumâ€“Oxygen Clusters in Reactions of Aln+ with Oxygen. Journal of Physical Chemistry A, 2019, 123, 7463-7469.	2.5	7
81	Multiple-Valence Aluminum and the Electronic and Geometric Structure of Al_{<i>n</i>}O_{<i>m</i>} Clusters. Journal of Physical Chemistry A, 2019, 123, 5114-5121.	2.5	7
82	[As₇M(CO)₃]^{3â€“} M = Cr, Mo, W: Bonding and Electronic Structure of Cluster Assemblies with Metal Carbonyls. Journal of Physical Chemistry C, 2011, 115, 23704-23710.	3.1	6
83	Interfacial magnetism in a fused superatomic cluster [Co₆Se₈(PEt₃)₅]₂. Nanoscale, 2021, 13, 15763-15769.	5.6	6
84	Quantum spin transport through magnetic superatom dimer (Cs8V-Cs8V). Journal of Chemical Physics, 2012, 137, 164311.	3.0	5
85	The effect of chalcogen and metal on the electronic properties and stability of metalâ€“chalcogenides clusters, TM6Xn(PH3)6 (TM = Mo, Cr, Re, Co, Ni; X = Se, Te; n = 8,5). European Physical Journal D, 2018, 72, 1.	1.3	5
86	Unusually large spin polarization and magnetoresistance in a FeMg8â€“FeMg8 superatomic dimer. Journal of Chemical Physics, 2013, 139, 064306.	3.0	4
87	Superatoms. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, 1, 365-381.	0.6	3
88	Stable magnetic order and charge induced rotation of magnetization in nano-clusters. Applied Physics Letters, 2014, 105, 152409.	3.3	2
89	On the enhancement of magnetic anisotropy in cobalt clusters via non-magnetic doping. Journal of Physics Condensed Matter, 2014, 26, 125303.	1.8	2
90	The structure and stability of CrnTem (1â€¯â‰¤â€¯nâ€¯â‰¤â€¯6, 1â€¯â‰¤â€¯mâ€¯â‰¤â€¯8) clusters. Chemical Physics Letters, 2019, 720 76-82.	2.6	1

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91	Creating Genetic Materials of Metal Clusters. , 2020, , 241-264.		1
92	Instrumentation for Cluster Science. , 2020, , 11-38.		0
93	Charge Transfer and the Harpoon Mechanism. , 2020, , 193-213.		0
94	Cooperative Active-Sites Mechanism. , 2020, , 81-95.		0
95	Metal Cluster Reacting with Oxygen. , 2020, , 39-56.		0
96	An Overview of Metal Clusters and Their Reactivity. , 2020, , 1-9.		0
97	Cluster Dissociation, Intracluster Reactivity and Effect of the Ligands. , 2020, , 175-191.		0