

# Shiv N Khanna

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/11276641/publications.pdf>

Version: 2024-02-01

97  
papers

5,333  
citations

126907

33  
h-index

82547

72  
g-index

99  
all docs

99  
docs citations

99  
times ranked

3665  
citing authors

#	ARTICLE	IF	CITATIONS
1	High-Spin Superatom Stabilized by Dual Subshell Filling. Journal of the American Chemical Society, 2022, 144, 5172-5179.	13.7	8
2	Interfacial magnetism in a fused superatomic cluster [Co <sub>6</sub> Se <sub>8</sub> (PEt <sub>3</sub> ) <sub>5</sub> ] <sub>2</sub> . Nanoscale, 2021, 13, 15763-15769.	5.6	6
3	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
4	The superatomic state beyond conventional magic numbers: Ligated metal chalcogenide superatoms. Journal of Chemical Physics, 2021, 155, 120901.	3.0	9
5	Creating Genetic Materials of Metal Clusters. , 2020, , 241-264.		1
6	Metal Clusters and Their Reactivity. , 2020, , .		9
7	Superatomic molecules with internal electric fields for light harvesting. Nanoscale, 2020, 12, 4736-4742.	5.6	15
8	Instrumentation for Cluster Science. , 2020, , 11-38.		0
9	Charge Transfer and the Harpoon Mechanism. , 2020, , 193-213.		0
10	Cooperative Active-Sites Mechanism. , 2020, , 81-95.		0
11	Metal Cluster Reacting with Oxygen. , 2020, , 39-56.		0
12	An Overview of Metal Clusters and Their Reactivity. , 2020, , 1-9.		0
13	Cluster Dissociation, Intracluster Reactivity and Effect of the Ligands. , 2020, , 175-191.		0
14	Al Valence Controls the Coordination and Stability of Cationic Aluminum-Oxygen Clusters in Reactions of Al <sub>n</sub> <sup>+</sup> with Oxygen. Journal of Physical Chemistry A, 2019, 123, 7463-7469.	2.5	7
15	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
16	Tuning the electronic properties of hexanuclear cobalt sulfide superatoms via ligand substitution. Chemical Science, 2019, 10, 1760-1766.	7.4	24
17	Multiple-Valence Aluminum and the Electronic and Geometric Structure of Al <sub>n</sub> O <sub>m</sub> Clusters. Journal of Physical Chemistry A, 2019, 123, 5114-5121.	2.5	7
18	The structure and stability of Cr <sub>n</sub> Te <sub>m</sub> (1 ≤ n ≤ 6, 1 ≤ m ≤ 8) clusters. Chemical Physics Letters, 2019, 720, 76-82.	2.6	1

#	ARTICLE	IF	CITATIONS
19	The effect of chalcogen and metal on the electronic properties and stability of metal-chalcogenides clusters, $TM_6X_n(PH_3)_6$ (TM = Mo, Cr, Re, Co, Ni; X = Se, Te; n = 8,5). European Physical Journal D, 2018, 72, 1.	1.3	5
20	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
21	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
22	Strong lowering of ionization energy of metallic clusters by organic ligands without changing shell filling. Nature Communications, 2018, 9, 2357.	12.8	34
23	Electronic and magnetic properties of $Fe_2Si_n$ ( $1 \leq n \leq 12$ ) clusters. Chemical Physics Letters, 2018, 706, 113-119.	2.6	11
24	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
25	Superatoms: Electronic and Geometric Effects on Reactivity. Accounts of Chemical Research, 2017, 50, 255-263.	15.6	203
26	Ionic versus metallic bonding in $Al_nM_m$ and $Al_nM_m$ ( $m \leq 3, n + m \leq 15$ ) clusters. Journal of Chemical Physics, 2017, 146, 224301.	3.0	17
27	Evolution of the Spin Magnetic Moments and Atomic Valence of Vanadium in $VCu_x$ , $VAg_x$ , and $VAu_x$ Clusters ( $x = 3-14$ ). Journal of Physical Chemistry A, 2017, 121, 2990-2999.	2.5	31
28	Effect of Embedding Platinum Clusters in Alumina on Sintering, Coking, and Activity. Journal of Physical Chemistry C, 2017, 121, 21527-21534.	3.1	9
29	CO ligands stabilize metal chalcogenide $Co_6Se_8(CO)_n$ clusters via demagnetization. Physical Chemistry Chemical Physics, 2017, 19, 31940-31948.	2.8	11
30	Complete $Ag_4M_2(DMSA)_4$ ( $M = Ni, Pd, Pt, DMSA =$ ) Characterization. Journal of Physical Chemistry A, 2017, 121, 5324-5331.	2.5	10
31	Transforming $Ni_9Te_6$ from Electron Donor to Acceptor via Ligand Exchange. Journal of Physical Chemistry A, 2016, 120, 6644-6649.	2.5	20
32	Reactivity of Metal Clusters. Chemical Reviews, 2016, 116, 14456-14492.	47.7	359
33	What determines if a ligand activates or passivates a superatom cluster?. Chemical Science, 2016, 7, 3067-3074.	7.4	67
34	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
35	$Ni_9Te_6(PEt_3)_8C_{60}$ Is a Superatomic Superalkali Superparamagnetic Cluster Assembled Material ( $S^3$ -CAM). Journal of the American Chemical Society, 2016, 138, 1916-1921.	13.7	42
36	Making sense of the conflicting magic numbers in $WSi_n$ clusters. Journal of Chemical Physics, 2015, 143, 074310.	3.0	13

#	ARTICLE	IF	CITATIONS
37	The Effects of Alkaline-Earth Counterions on the Architectures, Band-Gap Energies, and Proton Transfer of Triazole-Based Coordination Polymers. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 2085-2091.	2.0	8
38	Geometry controls the stability of FeSi <sub>14</sub> . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15718-15724.	2.8	21
39	Electronic structure, stability, and oxidation of boron-magnesium clusters and cluster solids. <i>Journal of Chemical Physics</i> , 2015, 142, 054304.	3.0	17
40	Atom precise platinum- $\mu$ -thiol crowns. <i>Nanoscale</i> , 2015, 7, 19448-19452.	5.6	12
41	IN QUEST OF A SYSTEMATIC FRAMEWORK FOR UNIFYING AND DEFINING NANOSCIENCE. <i>Modern Physics Letters B</i> , 2014, 28, 1430002.	1.9	17
42	Stable magnetic order and charge induced rotation of magnetization in nano-clusters. <i>Applied Physics Letters</i> , 2014, 105, 152409.	3.3	2
43	On the enhancement of magnetic anisotropy in cobalt clusters via non-magnetic doping. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 125303.	1.8	2
44	Nature of Valence Transition and Spin Moment in Ag <sub>n</sub> V <sup>+</sup> Clusters. <i>Journal of the American Chemical Society</i> , 2014, 136, 8229-8236.	13.7	53
45	Boron Substitution in Aluminum Cluster Anions: Magic Clusters and Reactivity with Oxygen. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8485-8492.	2.5	24
46	Does the 18-Electron Rule Apply to CrSi <sub>12</sub> ?. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3492-3496.	4.6	56
47	Reactivity of Silver Clusters Anions with Ethanethiol. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8345-8350.	2.5	12
48	The Oblate Structure and Unexpected Resistance in Reactivity of Ag <sub>15</sub> <sup>+</sup> with O <sub>2</sub> . <i>Journal of Physics: Conference Series</i> , 2013, 438, 012002.	0.4	12
49	Unusually large spin polarization and magnetoresistance in a FeMg <sub>8</sub> FeMg <sub>8</sub> superatomic dimer. <i>Journal of Chemical Physics</i> , 2013, 139, 064306.	3.0	4
50	Magnetic properties of Co <sub>2</sub> TMxC and Co <sub>3</sub> TMxC nanoparticles. <i>Journal of Applied Physics</i> , 2013, 114, 243909.	2.5	7
51	Electronic subshell splitting controls the atomic structure of charged and neutral silver clusters. <i>New Journal of Chemistry</i> , 2013, 37, 3928.	2.8	36
52	Synthesis and Structural Characterization of an Atom-Precise Bimetallic Nanocluster, Ag <sub>4</sub> Ni <sub>2</sub> (DMSA) <sub>4</sub> . <i>Journal of the American Chemical Society</i> , 2013, 135, 26-29.	13.7	51
53	On the Existence of Designer Magnetic Superatoms. <i>Journal of the American Chemical Society</i> , 2013, 135, 4856-4861.	13.7	108
54	Controlling the Band Gap Energy of Cluster-Assembled Materials. <i>Accounts of Chemical Research</i> , 2013, 46, 2385-2395.	15.6	81

#	ARTICLE	IF	CITATIONS
55	Robust Magnetic Moments on Impurities in Metallic Clusters: Localized Magnetic States in Superatoms. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4297-4303.	2.5	16
56	Probing the Magic Numbers of Aluminum-Magnesium Cluster Anions and Their Reactivity toward Oxygen. <i>Journal of the American Chemical Society</i> , 2013, 135, 4307-4313.	13.7	88
57	Spin Accommodation and Reactivity of Silver Clusters with Oxygen: The Enhanced Stability of $\text{Ag}_{13}^+$ . <i>Journal of the American Chemical Society</i> , 2012, 134, 18973-18978.	13.7	114
58	Ligand-Induced Active Sites: Reactivity of Iodine-Protected Aluminum Superatoms with Methanol. <i>Journal of the American Chemical Society</i> , 2012, 134, 20507-20512.	13.7	46
59	Synthesis, structure and band gap energy of covalently linked cluster-assembled materials. <i>Dalton Transactions</i> , 2012, 41, 12365.	3.3	33
60	Metallic and molecular orbital concepts in $\text{XMg}_8$ clusters, X = Be-F. <i>Journal of Chemical Physics</i> , 2012, 136, 134311.	3.0	14
61	Palladium in the Gap: Cluster Assemblies with Band Edges Localized on Linkers. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10207-10214.	3.1	9
62	Quantum spin transport through magnetic superatom dimer ( $\text{Cs}_8\text{V}-\text{Cs}_8\text{V}$ ). <i>Journal of Chemical Physics</i> , 2012, 137, 164311.	3.0	5
63	Magnetism of electrons in atoms and superatoms. <i>Journal of Applied Physics</i> , 2012, 112, 064313.	2.5	17
64	Magnetic properties of $\text{Co}_2\text{C}$ and $\text{Co}_3\text{C}$ nanoparticles and their assemblies. <i>Applied Physics Letters</i> , 2012, 101, .	3.3	64
65	Edge-Induced Active Sites Enhance the Reactivity of Large Aluminum Cluster Anions with Alcohols. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8085-8091.	2.5	41
66	Shell magnetism in transition metal doped calcium superatom. <i>Chemical Physics Letters</i> , 2012, 528, 39-43.	2.6	28
67	The Zintl ion $[\text{As}_7]^{2-}$ : an example of an electron-deficient $\text{As}_x$ radical anion. <i>Chemical Communications</i> , 2011, 47, 3126.	4.1	18
68	$[\text{As}_7\text{M}(\text{CO})_3]^+$ M = Cr, Mo, W: Bonding and Electronic Structure of Cluster Assemblies with Metal Carbonyls. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23704-23710.	3.1	6
69	On the Ground State of $\text{Pd}_{13}$ . <i>Journal of the American Chemical Society</i> , 2011, 133, 12192-12196.	13.7	74
70	Closed-shell to split-shell stability of isovalent clusters. <i>Physical Review B</i> , 2011, 84, .	3.2	7
71	Preparation of Elemental Cu and Ni Nanoparticles by the Polyol Method: An Experimental and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2656-2664.	3.1	217
72	Hund's rule in superatoms with transition metal impurities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 10062-10066.	7.1	105

#	ARTICLE	IF	CITATIONS
73	Stability and electronic properties of isoelectronic heteroatomic analogs of. Chemical Physics Letters, 2011, 505, 92-95.	2.6	8
74	Cooperative effects in the oxidation of CO by palladium oxide cations. Journal of Chemical Physics, 2011, 135, 234303.	3.0	18
75	Controlling Band Gap Energies in Cluster-Assembled Ionic Solids through Internal Electric Fields. ACS Nano, 2010, 4, 5813-5818.	14.6	72
76	Resilient aromaticity in lead–indium clusters. Chemical Physics Letters, 2010, 500, 196-201.	2.6	13
77	Crystal field effects on the reactivity of aluminum-copper cluster anions. Physical Review B, 2010, 81, .	3.2	59
78	Reactivity of Aluminum Cluster Anions with Water: Origins of Reactivity and Mechanisms for H <sub>2</sub> Release. Journal of Physical Chemistry A, 2010, 114, 6071-6081.	2.5	95
79	Anion Photoelectron Spectroscopy and First-Principles Study of Pb <sub>x</sub> In <sub>y</sub> Clusters. Journal of Physical Chemistry C, 2010, 114, 20907-20916.	3.1	15
80	Effect of Electronic and Geometric Shell Closures on the Stability of Neutral and Anionic TiNa <sub>n</sub> (n = 1–13) Clusters. Journal of Physical Chemistry C, 2010, 114, 10739-10744.	3.1	26
81	Cluster-Assembled Materials: Toward Nanomaterials with Precise Control over Properties. ACS Nano, 2010, 4, 235-240.	14.6	127
82	The applicability of three-dimensional aromaticity in BiSnn <sup>+</sup> Zintl analogues. Journal of Chemical Physics, 2010, 133, 134302.	3.0	17
83	Combined Experimental and Theoretical Study of Al <sub>n</sub> X (n = 1–6; X = As, Sb) Clusters: Evidence of Aromaticity and the Jellium Model. Journal of Physical Chemistry A, 2010, 114, 2045-2052.	2.5	23
84	Superatoms. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, 1, 365-381.	0.6	3
85	Designer magnetic superatoms. Nature Chemistry, 2009, 1, 310-315.	13.6	223
86	Helical and linear [K(As <sub>11</sub> ) <sub>2</sub> ] <sup>+</sup> chains: Role of solvent on the conformation of chains formed by Zintl anions. Chemical Physics Letters, 2009, 473, 305-311.	2.6	11
87	Highly efficient (Cs <sub>8</sub> V) superatom-based spin-polarizer. Applied Physics Letters, 2009, 95, .	3.3	26
88	Cluster-Assembled Materials. ACS Nano, 2009, 3, 244-255.	14.6	598
89	Complementary Active Sites Cause Size-Selective Reactivity of Aluminum Cluster Anions with Water. Science, 2009, 323, 492-495.	12.6	262
90	From SiO Molecules to Silicates in Circumstellar Space: Atomic Structures, Growth Patterns, and Optical Signatures of Si <sub>n</sub> O <sub>m</sub> Clusters. ACS Nano, 2008, 2, 1729-1737.	14.6	45

#	ARTICLE	IF	CITATIONS
91	Al <sub>n</sub> Bi Clusters: Transitions Between Aromatic and Jellium Stability. Journal of Physical Chemistry A, 2008, 112, 13316-13325.	2.5	29
92	Effect of Charge and Composition on the Structural Fluxionality and Stability of Nine Atom Tin <sup>+</sup> Bismuth Zintl Analogues. Inorganic Chemistry, 2008, 47, 10953-10958.	4.0	22
93	Superatom Compounds, Clusters, and Assemblies: Ultra Alkali Motifs and Architectures. Journal of the American Chemical Society, 2007, 129, 10189-10194.	13.7	186
94	Spin Accommodation and Reactivity of Aluminum Based Clusters with O <sub>2</sub> . Journal of the American Chemical Society, 2007, 129, 16098-16101.	13.7	147
95	From Designer Clusters to Synthetic Crystalline Nanoassemblies. Nano Letters, 2007, 7, 2734-2741.	9.1	109
96	Reactions of Al <sub>n</sub> X <sub>n</sub> -with Methyl Iodide: The Enhanced Stability of Al <sub>7</sub> I and the Chemical Significance of Active Centers. Journal of the American Chemical Society, 2005, 127, 16048-16053.	13.7	46
97	Formation of Al <sub>13</sub> I <sup>-</sup> : Evidence for the Superhalogen Character of Al <sub>13</sub> . Science, 2004, 304, 84-87.	12.6	515