

Puru Jena

List of Publications by Year in descending order

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625
papers

30,178
citations

5248

83
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9073

144
g-index

650
all docs

650
docs citations

650
times ranked

17442
citing authors

#	ARTICLE	IF	CITATIONS
1	Penta-graphene: A new carbon allotrope. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2372-2377.	3.3	1,114
2	Materials for Hydrogen Storage: Past, Present, and Future. Journal of Physical Chemistry Letters, 2011, 2, 206-211.	2.1	818
3	Ferromagnetism in Semihydrogenated Graphene Sheet. Nano Letters, 2009, 9, 3867-3870.	4.5	771
4	Clustering of Ti on a C60Surface and Its Effect on Hydrogen Storage. Journal of the American Chemical Society, 2005, 127, 14582-14583.	6.6	675
5	Assembling crystals from clusters. Physical Review Letters, 1992, 69, 1664-1667.	2.9	574
6	First-Principles Study of Hydrogen Storage on Li12C60. Journal of the American Chemical Society, 2006, 128, 9741-9745.	6.6	533
7	Hydrogen interactions with defects in crystalline solids. Reviews of Modern Physics, 1992, 64, 559-617.	16.4	471
8	Atomic clusters: Building blocks for a class of solids. Physical Review B, 1995, 51, 13705-13716.	1.1	432
9	Structures and Phase Transition of a MoS ₂ Monolayer. Journal of Physical Chemistry C, 2014, 118, 1515-1522.	1.5	432
10	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. Chemical Reviews, 2018, 118, 5755-5870.	23.0	426
11	Vacancy-induced magnetism in ZnO thin films and nanowires. Physical Review B, 2008, 77, .	1.1	409
12	Evolution of the electronic structure and properties of neutral and charged aluminum clusters: A comprehensive analysis. Journal of Chemical Physics, 1999, 111, 1890-1904.	1.2	332
13	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. Physical Review B, 2010, 81, .	1.1	278
14	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. Physical Chemistry Chemical Physics, 2016, 18, 8777-8784.	1.3	273
15	Beyond the Periodic Table of Elements: The Role of Superatoms. Journal of Physical Chemistry Letters, 2013, 4, 1432-1442.	2.1	248
16	Magic Numbers in Metallo-Inorganic Clusters: Chromium Encapsulated in Silicon Cages. Physical Review Letters, 2002, 89, 016803.	2.9	243
17	Electric field enhanced hydrogen storage on polarizable materials substrates. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 2801-2806.	3.3	221
18	Binding of hydrogen molecules by a transition-metal ion. Physical Review Letters, 1992, 68, 2277-2280.	2.9	220

#	ARTICLE	IF	CITATIONS
19	Electronic Structure and Properties of Transition Metal π -Benzene Complexes. <i>Journal of the American Chemical Society</i> , 2001, 123, 3799-3808.	6.6	219
20	Clusters: A bridge across the disciplines of physics and chemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 10560-10569.	3.3	218
21	Direct Observation of Key Reaction Intermediates on Gold Clusters. <i>Journal of the American Chemical Society</i> , 2003, 125, 2848-2849.	6.6	206
22	π -Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3234-3241.	2.1	205
23	Potential of AlN Nanostructures as Hydrogen Storage Materials. <i>ACS Nano</i> , 2009, 3, 621-626.	7.3	201
24	Carbon Nanomaterials as Catalysts for Hydrogen Uptake and Release in NaAlH ₄ . <i>Nano Letters</i> , 2009, 9, 1501-1505.	4.5	200
25	Electronic structures and bonding of graphyne sheet and its BN analog. <i>Journal of Chemical Physics</i> , 2011, 134, 174701.	1.2	182
26	The Intrinsic Ferromagnetism in a MnO ₂ Monolayer. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3382-3386.	2.1	171
27	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6055-6059.	1.5	171
28	Unexpected Stability of Al ₄ H ₆ : A Borane Analog?. <i>Science</i> , 2007, 315, 356-358.	6.0	169
29	Spin Conservation Accounts for Aluminum Cluster Anion Reactivity Pattern with O ₂ . <i>Science</i> , 2008, 319, 438-442.	6.0	168
30	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. <i>Nano Letters</i> , 2015, 15, 8277-8281.	4.5	168
31	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN ₂ Sheet. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3993-3998.	1.5	167
32	Physics of small metal clusters: Topology, magnetism, and electronic structure. <i>Physical Review B</i> , 1985, 32, 2058-2069.	1.1	157
33	Systematic Study of Oxo, Peroxo, and Superoxo Isomers of 3d-Metal Dioxides and Their Anions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11961-11971.	1.1	151
34	Hyperhalogens: Discovery of a New Class of Highly Electronegative Species. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8966-8970.	7.2	146
35	Three-Dimensional Metallic Boron Nitride. <i>Journal of the American Chemical Society</i> , 2013, 135, 18216-18221.	6.6	145
36	Giant Magnetic Moments of Nitrogen-Doped Mn Clusters and their Relevance to Ferromagnetism in Mn-Doped GaN. <i>Physical Review Letters</i> , 2002, 89, 185504.	2.9	144

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37	Optical properties of Ti ₃ SiC ₂ and Ti ₄ AlN ₃ . Applied Physics Letters, 2008, 92, .	1.5	143
38	Stable three-dimensional metallic carbon with interlocking hexagons. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18809-18813.	3.3	134
39	Hydrogen storage and the 18-electron rule. Journal of Chemical Physics, 2006, 124, 224703.	1.2	133
40	Origin of the unusual stability of MnO ₄ ²⁻ . Chemical Physics Letters, 1999, 312, 598-605.	1.2	132
41	Geometry and electronic structure of Vn(Bz) _m complexes. Journal of Chemical Physics, 2004, 120, 10414-10422.	1.2	130
42	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. Journal of Chemical Theory and Computation, 2009, 5, 374-379.	2.3	130
43	Magnetism and local order: Ab initio tight-binding theory. Physical Review B, 1989, 39, 6914-6924.	1.1	128
44	Electronic structure and magnetism of Rh _n (n=2-13) clusters. Physical Review B, 1999, 59, 5214-5222.	1.1	127
45	The rise of two-dimensional van der Waals ferroelectrics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1365.	6.2	127
46	Lattice thermal conductivity of penta-graphene. Carbon, 2016, 105, 424-429.	5.4	120
47	Superalkalis and Superhalogens As Building Blocks of Supersalts. Journal of Physical Chemistry A, 2014, 118, 638-645.	1.1	119
48	Atomic and electronic structure of neutral and charged Si _n O _m clusters. Journal of Chemical Physics, 1998, 109, 1245-1250.	1.2	118
49	Superhalogens as Building Blocks of Halogen-Free Electrolytes in Lithium-Ion Batteries. Angewandte Chemie - International Edition, 2014, 53, 13916-13919.	7.2	117
50	Electronic structure of chromium oxides, CrO _n ²⁺ and CrO _n (n=1-5) from photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2001, 115, 7935-7944.	1.2	115
51	Anomalous magnetism in small Mn clusters. Chemical Physics Letters, 1998, 289, 473-479.	1.2	114
52	Structure and bonding of Au ₅ M (M=Na, Mg, Al, Si, P, and S) clusters. Physical Review B, 2006, 74, .	1.1	113
53	Carrier-mediated ferromagnetism in N codoped (Zn,Mn)O(101 $\bar{1}$ 0) thin films. Physical Review B, 2004, 70, .	1.1	112
54	Magnetism in small vanadium clusters. Physical Review B, 1991, 43, 8179-8182.	1.1	111

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55	Physics of Nickel Clusters. 2. Electronic Structure and Magnetic Properties. Journal of Physical Chemistry A, 1998, 102, 1748-1759.	1.1	110
56	Quantum anomalous Hall effect in ferromagnetic transition metal halides. Physical Review B, 2017, 95, .	1.1	110
57	Appearance of bulk properties in small tungsten oxide clusters. Journal of Chemical Physics, 2004, 121, 9417-9422.	1.2	109
58	Interactions of Au cluster anions with oxygen. Journal of Chemical Physics, 2004, 120, 6510-6515.	1.2	107
59	Li-rich antiperovskite superionic conductors based on cluster ions. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11046-11051.	3.3	107
60	Temperature Dependence of Electric Field Gradients in Noncubic Metals. Physical Review Letters, 1976, 36, 418-421.	2.9	106
61	Storage of Molecular Hydrogen in B ⁺ N Cage: Energetics and Thermal Stability. Nano Letters, 2005, 5, 1273-1277.	4.5	106
62	Electronic structure of hydrogen in simple metals. Physical Review B, 1978, 17, 3518-3524.	1.1	105
63	Electronic, Magnetic, and Geometric Structure of Metallo-Carbohedrenes. Science, 1992, 258, 1640-1643.	6.0	105
64	Physics of Nickel Clusters: Energetics and Equilibrium Geometries. Journal of Physical Chemistry A, 1997, 101, 1072-1080.	1.1	103
65	Mechanistic Insight into Photocatalytic Pathways of MIL-100(Fe)/TiO ₂ Composites. ACS Applied Materials & Interfaces, 2019, 11, 12516-12524.	4.0	103
66	Electronic Structure of the 3d Metal Monoxide Anions. Journal of Physical Chemistry A, 2000, 104, 5374-5379.	1.1	102
67	Unique magnetic signature of transition metal atoms supported on benzene. Chemical Physics Letters, 2000, 321, 142-150.	1.2	101
68	Superhalogen Properties of Fluorinated Coinage Metal Clusters. Journal of Physical Chemistry C, 2010, 114, 16018-16024.	1.5	101
69	Hydroxyl-decorated graphene systems as candidates for organic metal-free ferroelectrics, multiferroics, and high-performance proton battery cathode materials. Physical Review B, 2013, 87, .	1.1	100
70	Ferromagnetism in Mn-Doped GaN Nanowires. Physical Review Letters, 2005, 95, 167202.	2.9	96
71	Atomic and electronic structures of neutral and charged boron and boron-rich clusters. Journal of Chemical Physics, 1997, 107, 132-140.	1.2	95
72	Highly selective CO ₂ /CH ₄ gas uptake by a halogen-decorated borazine-linked polymer. Journal of Materials Chemistry, 2012, 22, 13524.	6.7	95

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73	Designing ionic solids from metallic clusters. <i>Chemical Physics Letters</i> , 1994, 219, 479-483.	1.2	91
74	Ferromagnetism in small clusters. <i>Physical Review Letters</i> , 1991, 66, 938-941.	2.9	90
75	Anomalous Behavior of Atomic Hydrogen Interacting with Gold Clusters. <i>Journal of the American Chemical Society</i> , 2003, 125, 14205-14209.	6.6	90
76	Closo-alanes (Al ₄ H ₄ , Al _n H _{n+2} , 4 ≤ n ≤ 8): A New Chapter in Aluminum Hydride Chemistry. <i>Journal of the American Chemical Society</i> , 2007, 129, 5969-5975.	6.6	90
77	Review of modification strategies in emerging inorganic solid-state electrolytes for lithium, sodium, and potassium batteries. <i>Joule</i> , 2022, 6, 543-587.	11.7	90
78	Electronic signature of the magicity and ionic bonding in Al ₁₃ X (X=Li, K) clusters. <i>Physical Review B</i> , 2002, 65, .	1.1	89
79	Role of catalysts in dehydrogenation of MgH ₂ nanoclusters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 8227-8231.	3.3	89
80	Functionalized heterofullerenes for hydrogen storage. <i>Applied Physics Letters</i> , 2009, 94, .	1.5	89
81	Equilibrium Geometry, Stability, and Magnetic Properties of Small MnO Clusters. <i>Journal of the American Chemical Society</i> , 1999, 121, 644-652.	6.6	88
82	Stabilization of Si ₆₀ Cage Structure. <i>Physical Review Letters</i> , 2003, 90, 135503.	2.9	88
83	Clusters: A bridge across the disciplines of environment, materials science, and biology. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 10554-10559. Magnetic properties of transition-metal-doped	3.3	88
84			

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91	Relationship between magnetism, topology, and reactivity of Rh clusters. <i>Physical Review B</i> , 1997, 56, 8849-8854.	1.1	81
92	AlH ₃ and Al ₂ H ₆ : Magic Clusters with Unmagical Properties. <i>Physical Review Letters</i> , 2001, 86, 692-695.	2.9	81
93	Vacancy-mediated hydrogen desorption in NaAlH ₄ . <i>Physical Review B</i> , 2005, 72, .	1.1	81
94	Manganese-Based Magnetic Superhalogens. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 2568-2572.	7.2	81
95	Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes. <i>Physical Review B</i> , 2011, 84, .	1.1	81
96	Magic Rule for Al _n H _m Magic Clusters. <i>Physical Review Letters</i> , 2007, 98, 256802.	2.9	80
97	Exceptional Thermoelectric Properties of Layered GeAs ₂ . <i>Chemistry of Materials</i> , 2017, 29, 9300-9307.	3.2	80
98	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3501-3506.	2.1	80
99	Spontaneous fragmentation of multiply charged metal clusters. <i>Physical Review Letters</i> , 1987, 58, 1188-1191.	2.9	79
100	Interaction of H ₂ and He with metal atoms, clusters, and ions. <i>Physical Review B</i> , 1995, 51, 4475-4484.	1.1	78
101	Borane Derivatives: A New Class of Super- and Hyperhalogens. <i>ChemPhysChem</i> , 2011, 12, 2423-2428.	1.0	77
102	Enhanced Carbon Dioxide Capture from Landfill Gas Using Bifunctionalized Benzimidazole-Linked Polymers. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 14648-14655.	4.0	76
103	Lithium-doped triazine-based graphitic C ₃ N ₄ sheet for hydrogen storage at ambient temperature. <i>Computational Materials Science</i> , 2014, 81, 275-279.	1.4	75
104	Single Pd atoms in activated carbon fibers and their contribution to hydrogen storage. <i>Carbon</i> , 2011, 49, 4050-4058.	5.4	74
105	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. <i>Scientific Reports</i> , 2015, 5, 14342.	1.6	74
106	Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI ₃ Monolayer through van der Waals Heterostructures. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17987-17993.	1.5	74
107	Electronic Structure and Properties of FeO and FeO _n -Clusters. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5812-5822.	1.1	72
108	Stability of B ₁₂ (CN) ₁₂ ²⁺ : Implications for Lithium and Magnesium Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 3704-3708.	7.2	72

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109	Tetragonal C_{24} : a topological nodal-surface semimetal with potential as an anode material for sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 5733-5739.	5.2	72
110	Structure and stability of the AlX and AlX^+ species. <i>Journal of Chemical Physics</i> , 1999, 110, 2928-2935.	1.2	70
111	First-principles calculations of metal stabilized Si_2O cages. <i>Physical Review B</i> , 2002, 65, .	1.1	70
112	Periodic table of 3d-metal dimers and their ions. <i>Journal of Chemical Physics</i> , 2004, 121, 6785-6797.	1.2	70
113	Role of titanium in hydrogen desorption in crystalline sodium alanate. <i>Applied Physics Letters</i> , 2005, 86, 251913.	1.5	69
114	Comment on "Combinatorial Search for Optimal Hydrogen-Storage Nanomaterials Based on Polymers". <i>Physical Review Letters</i> , 2006, 97, 209601.	2.9	69
115	Theoretical Study of the Stability and Electronic Structure of $Al(BH_4)_n$ and $Al(BF_4)_n$ and Their Hyperhalogen Behavior. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10237-10243.	1.1	69
116	Ferromagnetism in Mn-doped GaN: From clusters to crystals. <i>Physical Review B</i> , 2003, 68, .	1.1	68
117	Clusters: A bridge between disciplines. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 10552-10553.	3.3	68
118	Interpretation of hyperfine fields in concentrated ferromagnetic alloys. <i>Solid State Communications</i> , 1974, 15, 139-142.	0.9	67
119	Isomerism and Novel Magnetic Order in Mn_{13} Cluster. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9853-9856.	1.1	67
120	Tuning magnetic properties of graphene nanoribbons with topological line defects: From antiferromagnetic to ferromagnetic. <i>Physical Review B</i> , 2012, 85, .	1.1	67
121	Giant Magnetic Moments and Magnetic Bistability of Stoichiometric MnO Clusters. <i>Physical Review Letters</i> , 1998, 81, 2970-2973.	2.9	66
122	Isomers of Al_{13} clusters and their interaction with alkali atoms. <i>Physical Review B</i> , 2000, 62, 4666-4671.	1.1	66
123	Quantum chemical study of adhesion at the SiC/Al interface. <i>Journal of Applied Physics</i> , 1988, 64, 6246-6253.	1.1	65
124	Body-Centered Tetragonal C_{16} : A Novel Topological Node-Line Semimetallic Carbon Composed of Tetrarings. <i>Small</i> , 2017, 13, 1602894.	5.2	65
125	Stability of Doubly Charged Transition-Metal Dimers. <i>Physical Review Letters</i> , 1987, 59, 2562-2565.	2.9	64
126	Competition between linear and cyclic structures in monochromium carbide clusters CrC_n^+ and $CrC_n^{\pm}(n=2-8)$: A photoelectron spectroscopy and density functional study. <i>Journal of Chemical Physics</i> , 2004, 120, 8996-9008.	1.2	64

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127	Structure and Properties of Fe _n , Fe _n ⁺ , and Fe _n ⁺ Clusters, $n = 7-20$. Journal of Physical Chemistry A, 2012, 116, 10218-10228.	1.1	64
128	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. Physical Review Letters, 2017, 119, 046403.	2.9	64
129	Electronic structure of substoichiometric Fe-Al intermetallics. Physical Review B, 2002, 66, .	1.1	63
130	Ferromagnetism in Cr-doped GaN: A first-principles calculation. Physical Review B, 2004, 69, .	1.1	63
131	Ab initio calculation of interatomic potentials and electronic properties of a simple metal-Al. Physical Review B, 1981, 24, 7057-7070.	1.1	62
132	Evolution of the electronic and structural properties of microclusters. Physical Review B, 1987, 36, 953-960.	1.1	62
133	Stability and magnetic properties of iron atoms encapsulated in Si clusters. Chemical Physics Letters, 2003, 373, 433-438.	1.2	62
134	Molecular Origin of Properties of Organic-Inorganic Hybrid Perovskites: The Big Picture from Small Clusters. Journal of Physical Chemistry Letters, 2016, 7, 1596-1603.	2.1	60
135	Evidence for a new class of solids. First-principles study of K(Al ₁₃). Chemical Physics Letters, 1996, 248, 213-217.	1.2	59
136	Experimental and theoretical study of the photoelectron spectra of MnO _x ⁺ ($x=1-3$) clusters. Journal of Chemical Physics, 2000, 113, 1473-1483.	1.2	59
137	Equilibrium structure and bonding of small iron-carbon clusters. Journal of Chemical Physics, 1996, 105, 11020-11023.	1.2	58
138	Energetics and electronic structure of carbon doped aluminum clusters. Journal of Chemical Physics, 2001, 115, 778-783.	1.2	58
139	Ferromagnetic and Half-Metallic FeC ₂ Monolayer Containing C ₂ Dimers. ACS Applied Materials & Interfaces, 2016, 8, 26207-26212.	4.0	58
140	Rational design of super-alkalis and their role in CO ₂ activation. Nanoscale, 2017, 9, 4891-4897.	2.8	58
141	FeO ₄ : A unique example of a closed-shell cluster mimicking a superhalogen. Physical Review A, 1999, 59, 3681-3684.	1.0	57
142	Magnetic coupling between Cr atoms doped at bulk and surface sites of ZnO. Applied Physics Letters, 2005, 87, 162509.	1.5	57
143	Theoretical study of deep-defect states in bulk PbTe and in thin films. Physical Review B, 2007, 76, .	1.1	57
144	Synthesis and characterization of highly porous borazine-linked polymers and their performance in hydrogen storage application. Journal of Materials Chemistry, 2011, 21, 10629.	6.7	57

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145	Equilibrium geometries, electronic structure and magnetic properties of small manganese clusters. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 10863-10877.	0.7	56
146	Antiferromagnetic Coupling Driven by Bond Length Contraction near the Ga _{1-x} Mn _x N Film Surface. <i>Physical Review Letters</i> , 2004, 93, 155501.	2.9	56
147	Magnetism and energetics of Mn-Doped ZnO(101̂0) thin films. <i>Physical Review B</i> , 2004, 69, .	1.1	56
148	Organozintl Clusters [P ₇ R ₄]: A New Class of Superalkalis. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 800-805.	2.1	56
149	Observation of a spin-protected high-energy isomer of Al ₄ N ⁻ cluster. <i>Chemical Physics Letters</i> , 1999, 301, 379-384.	1.2	55
150	Patterning Graphitic C ₆ N Sheets into a Kagome Lattice for Magnetic Materials. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 259-263.	2.1	55
151	Superhalogen-based lithium superionic conductors. <i>Journal of Materials Chemistry A</i> , 2017, 5, 13373-13381.	5.2	55
152	Au(CN) _n Complexes: Superhalogens with Pseudohalogen as Building Blocks. <i>Inorganic Chemistry</i> , 2011, 50, 8918-8925.	1.9	54
153	A systematic study of neutral and charged 3d-metal trioxides and tetraoxides. <i>Journal of Chemical Physics</i> , 2011, 134, 144305.	1.2	54
154	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3109-3114.	2.1	54
155	SiTe monolayers: Si-based analogues of phosphorene. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6353-6361.	2.7	54
156	Switendick criterion for stable hydrides. <i>Physical Review B</i> , 1985, 31, 6726-6730.	1.1	53
157	Magnetism and local order. II. Self-consistent cluster calculations. <i>Physical Review B</i> , 1989, 40, 399-406.	1.1	53
158	Models of electronic structure of hydrogen in metals: Pd-H. <i>Physical Review B</i> , 1979, 20, 3543-3551.	1.1	52
159	Electronic structure and geometries of heteroatomic clusters. <i>Physical Review B</i> , 1988, 37, 2867-2873.	1.1	52
160	Structure of SiAu ₁₆ : Can a silicon atom be stabilized in a gold cage?. <i>Journal of Chemical Physics</i> , 2007, 127, 214706.	1.2	52
161	Superhalogen properties of Cu _n clusters. <i>Journal of Chemical Physics</i> , 2009, 131, 124301.	1.2	52
162	Origin of the Unusual Stability of B ₁₂ and B ₁₃ ⁺ Clusters. <i>Inorganic Chemistry</i> , 2009, 48, 9965-9967.	1.9	52

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163	Electron Distribution around a Magnetic Impurity in a Nonmagnetic Host. <i>Physical Review B</i> , 1973, 7, 439-450.	1.1	51
164	Ferrimagnetism in Mn ₇ cluster. <i>Chemical Physics Letters</i> , 2003, 378, 374-379.	1.2	51
165	Electronic Structure and Bonding of Au on aSiO ₂ Cluster: A Nanobullet for Tumors. <i>Physical Review Letters</i> , 2004, 93, 186803.	2.9	51
166	Structures and photoelectron spectroscopy of Cu _n (BO ₂) _m ⁺ (n, m = 1, 2) clusters: Observation of hyperhalogen behavior. <i>Journal of Chemical Physics</i> , 2011, 134, 094309.	1.2	51
167	New insights into carbon dioxide interactions with benzimidazole-linked polymers. <i>Chemical Communications</i> , 2014, 50, 3571-3574.	2.2	51
168	(BaI ₂)Cs:mA cluster-assembled solid. <i>Physical Review B</i> , 1997, 55, 15868-15873.	1.1	50
169	Synthesis, Characterization, and Atomistic Modeling of Stabilized Highly Pyrophoric Al(BH ₄) ₃ via the Formation of the Hypersalt K[Al(BH ₄) ₄]. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19905-19915.	1.5	50
170	Alkalization of aluminum clusters. <i>Journal of Chemical Physics</i> , 2000, 113, 1508-1513.	1.2	49
171	Ferromagnetic GaN ⁺ Cr Nanowires. <i>Nano Letters</i> , 2005, 5, 1587-1590.	4.5	49
172	Effect of Au coating on the magnetic and structural properties of Fe nanoclusters for use in biomedical applications: A density-functional theory study. <i>Physical Review B</i> , 2006, 73, .	1.1	49
173	Negative ions of transition metal-halogen clusters. <i>Journal of Chemical Physics</i> , 2010, 133, 144301.	1.2	49
174	Multiferroic Materials Based on Organic Transition-Metal Molecular Nanowires. <i>Journal of the American Chemical Society</i> , 2012, 134, 14423-14429.	6.6	49
175	Aromatic Superhalogens. <i>Chemistry - A European Journal</i> , 2014, 20, 4736-4745.	1.7	49
176	Geometry, electronic structure, and energetics of copper-doped aluminum clusters. <i>Journal of Chemical Physics</i> , 2001, 114, 9792-9796.	1.2	48
177	Multidecker Organometallic Complexes for Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6181-6185.	1.5	48
178	A Recipe for Designing Molecules with Ever-Increasing Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1469-1474.	1.1	48
179	Density Functional Theory Study of the Interaction of Hydrogen with Li ₆ C ₆₀ . <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1084-1088.	2.1	48
180	Caging of Ni clusters by benzene molecules and its effect on the magnetism of Ni clusters. <i>Journal of Chemical Physics</i> , 2002, 116, 1343-1349.	1.2	47

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