

Puru Jena

List of Publications by Year in descending order

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625
papers

30,178
citations

5248

83
h-index

9073

144
g-index

650
all docs

650
docs citations

650
times ranked

17442
citing authors

#	ARTICLE	IF	CITATIONS
1	Metallo-boranes: a class of unconventional superhalogens defying electron counting rules. <i>Nanoscale</i> , 2022, 14, 1767-1778.	2.8	3
2	SbCl ₄ : An Exceptional Superhalogen as the Building Block of a Mixed Valence Supercrystal with Unconventional Ferroelectricity. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1049-1056.	2.1	6
3	Superatomic chemistry. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100350.	1.3	2
4	Halogen-Free Electrolytes Based on Modified Boranes for Alkali-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5112-5121.	1.5	2
5	Atomically Precise Core-Tailored Metal Chalcogenide Nanoclusters: Tuning the Electronic Structure and Magnetic Properties. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6512-6522.	1.5	3
6	Interfacial triferroicity in monolayer chromium dihalide. <i>Physical Review B</i> , 2022, 105, .	1.1	5
7	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
8	Argyrodite-type advanced lithium conductors and transport mechanisms beyond paddle-wheel effect. <i>Nature Communications</i> , 2022, 13, 2078.	5.8	27
9	Reply to the "Comment on "Realization of the Zn ³⁺ oxidation state" by Y. Shang, N. Shu, Z. Zhang, P. Yang and J. Xu, <i>Nanoscale</i> , 2022, 14, DOI: 10.1039/D1NR07031B. <i>Nanoscale</i> , 2022, 14, 8881-8885.	2.8	0
10	NaNO_3 monolayer: A stable graphenelike supersalt with strong four-phonon scattering and low lattice thermal conductivity insensitive to temperature. <i>Physical Review Materials</i> , 2022, 6, .	0.9	8
11	Halide sublattice dynamics drive Li-ion transport in antiperovskites. <i>Journal of Materials Chemistry A</i> , 2022, 10, 15731-15742.	5.2	3
12	Designing New Metal Chalcogenide Nanoclusters through Atom-by-Atom Substitution. <i>Small</i> , 2021, 17, e2002927.	5.2	7
13	Two-dimensional metal-free boron chalcogenides B ₂ X ₃ (X = Se and Te) as photocatalysts for water splitting under visible light. <i>Nanoscale</i> , 2021, 13, 3627-3632.	2.8	9
14	Imidazole-graphyne: a new 2D carbon nitride with a direct bandgap and strong IR refraction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10274-10280.	1.3	4
15	A family of ionic supersalts with covalent-like directionality and unconventional multiferroicity. <i>Nature Communications</i> , 2021, 12, 1331.	5.8	19
16	Built-in electric field control of magnetic coupling in van der Waals semiconductors. <i>Physical Review B</i> , 2021, 103, .	1.1	19
17	Role of Size and Composition on the Design of Superalkalis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5886-5894.	1.1	5
18	Binding of noble gas atoms by superhalogens. <i>Journal of Chemical Physics</i> , 2021, 155, 014304.	1.2	5

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19	Antiperovskite K_3OI for K-Ion Solid State Electrolyte. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7120-7126.	2.1	33
20	Theory-Guided Discovery of Novel Materials. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6499-6513.	2.1	11
21	Heavily Tungsten-Doped Sodium Thioantimonate Solid-State Electrolytes with Exceptionally Low Activation Energy for Ionic Diffusion. <i>Angewandte Chemie</i> , 2021, 133, 26362-26370.	1.6	2
22	Heavily Tungsten-Doped Sodium Thioantimonate Solid-State Electrolytes with Exceptionally Low Activation Energy for Ionic Diffusion. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 26158-26166.	7.2	18
23	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. <i>Carbon</i> , 2021, 183, 652-659.	5.4	10
24	Super-electrophiles of tri- and tetra-anions stabilized by selected terminal groups and their role in binding noble gas atoms. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21496-21500.	1.3	5
25	Realization of the Zn^{3+} oxidation state. <i>Nanoscale</i> , 2021, 13, 14041-14048.	2.8	13
26	Boron-Functionalized Organic Framework as a High-Performance Metal-Free Catalyst for N_2 Fixation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12142-12149.	2.1	9
27	Discovery of twin orbital-order phases in ferromagnetic semiconducting VI_3 monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 512-517.	1.3	29
28	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. <i>Journal of Power Sources</i> , 2020, 478, 228746.	4.0	14
29	Assembling Si_2BN nanoribbons into a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance. <i>Nanoscale</i> , 2020, 12, 19367-19374.	2.8	25
30	B_2H_6 splitting on catalytic surfaces and role of BH_3 towards hydrogen spillover. <i>Journal of Power Sources</i> , 2020, 455, 227973.	4.0	2
31	A 3D porous honeycomb carbon as Na-ion battery anode material with high capacity, excellent rate performance, and robust stability. <i>Carbon</i> , 2020, 168, 163-168.	5.4	25
32	Robustness of Superatoms and Their Potential as Building Blocks of Materials: Al_{13}^{+} vs $B(CN)_4^{+}$. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6435-6440.	1.5	7
33	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. <i>Physical Review Letters</i> , 2020, 124, 067602.	2.9	84
34	Clusters and Nanomaterials for Sustainable Energy. <i>ACS Energy Letters</i> , 2020, 5, 428-429.	8.8	4
35	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3501-3506.	2.1	80
36	Yttrium-Sodium Halides as Promising Solid-State Electrolytes with High Ionic Conductivity and Stability for Na-Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3376-3383.	2.1	43

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37	Record-high stability and compactness of multiply-charged clusters aided by selected terminal groups. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4880-4883.	1.3	7
38	Unique reactivity of B in B[Ge ₉ Y ₃] ₃ (Y = H, CH ₃ , BO,) <i>Tj ETQq000 rgBT/Overlock</i>	1.3	4
39	Hydrogenated C ₆₀ as High-Capacity Stable Anode Materials for Li Ion Batteries. <i>ACS Applied Energy Materials</i> , 2019, 2, 6453-6460.	2.5	19
40	Lattice Dynamic and Instability in Pentasilicene: A Light Single-Element Ferroelectric Material With High Curie Temperature. <i>Physical Review Applied</i> , 2019, 11, .	1.5	24
41	Stable Tetra- and Penta- Anions in the Gas Phase. <i>Angewandte Chemie</i> , 2019, 131, 11370-11374.	1.6	0
42	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
43	Rational Design of Porous Nodal-Line Semimetallic Carbon for K-Ion Battery Anode Materials. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6360-6367.	2.1	31
44	Boronated holey graphene: a case of 2D ferromagnetic metal. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21128-21135.	1.3	3
45	Ligand stabilization of manganocene dianions " in defiance of the 18-electron rule. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24300-24307.	1.3	6
46	Homocoupling and Heterocoupling of Grignard Perfluorobenzene Reagents via Aryne Intermediates: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9693-9700.	1.1	1
47	Conserved Vibrational Coherence in the Ultrafast Rearrangement of 2-Nitrotoluene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1140-1152.	1.1	24
48	A high-pressure induced stable phase of Li ₂ MnSiO ₄ as an effective poly-anion cathode material from simulations. <i>Journal of Materials Chemistry A</i> , 2019, 7, 16406-16413.	5.2	6
49	Tuning range-separated DFT functionals for modeling the peak absorption of MEH-PPV polymer in various solvents. <i>Computational and Theoretical Chemistry</i> , 2019, 1162, 112506.	1.1	33
50	Stable Tetra- and Penta- Anions in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11248-11252.	7.2	19
51	N-doped peanut-shaped carbon nanotubes for efficient CO ₂ electrocatalytic reduction. <i>Carbon</i> , 2019, 152, 241-246.	5.4	29
52	Rational Design of Stable Dianions and the Concept of Super-Chalcogens. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5753-5761.	1.1	10
53	Superhalogens as Building Blocks of Super Lewis Acids. <i>ChemPhysChem</i> , 2019, 20, 1607-1612.	1.0	11
54	Mechanistic Insight into Photocatalytic Pathways of MIL-100(Fe)/TiO ₂ Composites. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 12516-12524.	4.0	103

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55	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
56	Interfacial properties of penta-graphene-metal contacts. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	11
57	Stable Tetra- and Penta- Anions in the Gas Phase. <i>Angewandte Chemie</i> , 2019, 131, 11246.	1.6	0
58	Sodium Superionic Conductors Based on Clusters. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 963-972.	4.0	44
59	Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4350-4356.	1.1	4
60	Dissociation dynamics of 3- and 4-nitrotoluene radical cations: Coherently driven C-NO ₂ bond homolysis. <i>Journal of Chemical Physics</i> , 2018, 148, 134305.	1.2	17
61	A metallic peanut-shaped carbon nanotube and its potential for CO ₂ capture. <i>Carbon</i> , 2018, 132, 249-256.	5.4	13
62	Ultrafast coherent vibrational dynamics in dimethyl methylphosphonate radical cation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4636-4640.	1.3	11
63	Effect of hydrogenation on the structure and magnetic properties of an iron oxide cluster. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4546-4553.	1.3	11
64	Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metal-Organic Coordination Networks. <i>Advanced Electronic Materials</i> , 2018, 4, 1700323.	2.6	17
65	The rise of two-dimensional van der Waals ferroelectrics. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1365.	6.2	127
66	Co-mixing hydrogen and methane may double the energy storage capacity. <i>Journal of Materials Chemistry A</i> , 2018, 6, 8916-8922.	5.2	22
67	Simultaneous Detection and Removal of Formaldehyde at Room Temperature: Janus Au@ZnO@ZIF-8 Nanoparticles. <i>Nano-Micro Letters</i> , 2018, 10, 4.	14.4	84
68	Electron affinity of modified benzene. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25504.	1.0	18
69	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. <i>Carbon</i> , 2018, 127, 527-532.	5.4	32
70	B(SCN) ₄ ⁺ : A New Weakly Coordinating Anion in the Tetracyanoborate Family. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13371-13375.	1.5	5
71	Super-alkalis as building blocks of one-dimensional hierarchical electrides. <i>Nanoscale</i> , 2018, 10, 22963-22969.	2.8	13
72	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. <i>Chemical Reviews</i> , 2018, 118, 5755-5870.	23.0	426

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73	Collective Superexchange and Exchange Coupling Constants in the Hydrogenated Iron Oxide Particle $\text{Fe}_8\text{O}_{12}\text{H}_8$. Journal of Physical Chemistry A, 2018, 122, 5043-5049.	1.1	1
74	Discovery of a high-pressure phase of rutile-like CoO_2 and its potential as a cathode material. Journal of Materials Chemistry A, 2018, 6, 18449-18457.	5.2	9
75	A new 3D Dirac nodal-line semi-metallic graphene monolith for lithium ion battery anode materials. Journal of Materials Chemistry A, 2018, 6, 13816-13824.	5.2	44
76	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. Physical Review Materials, 2018, 2, .	0.9	21
77	Body-Centered Tetragonal C_{16} : A Novel Topological Node-Line Semimetallic Carbon Composed of Tetrarings. Small, 2017, 13, 1602894.	5.2	65
78	Two-dimensional topological crystalline quantum spin Hall effect in transition metal intercalated compounds. Physical Review B, 2017, 95, .	1.1	10
79	Rational design of super-alkalis and their role in CO_2 activation. Nanoscale, 2017, 9, 4891-4897.	2.8	58
80	Superhalogen-based lithium superionic conductors. Journal of Materials Chemistry A, 2017, 5, 13373-13381.	5.2	55
81	Rational Design of Stable Dianions by Functionalizing Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2017, 18, 1937-1942.	1.0	3
82	Role of ligands in the stability of B_nX_n and CB_nX_n ($n = 5-10$; X = H, F, CN) and their potential as building blocks of electrolytes in lithium ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 17937-17943.	1.3	24
83	$\text{B}_{12}(\text{SCN})_{12}$: An Ultrastable Weakly Coordinating Dianion. Journal of Physical Chemistry C, 2017, 121, 7697-7702.	1.5	31
84	Quantum anomalous Hall effect in ferromagnetic transition metal halides. Physical Review B, 2017, 95, .	1.1	110
85	A Theoretical and Mass Spectrometry Study of Dimethyl Methylphosphonate: New Isomers and Cation Decay Channels in an Intense Femtosecond Laser Field. Journal of Physical Chemistry A, 2017, 121, 8414-8424.	1.1	22
86	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
87	Exceptional Thermoelectric Properties of Layered GeAs_2 . Chemistry of Materials, 2017, 29, 9300-9307.	3.2	80
88	Colossal Stability of Gas-Phase Trianions: Superpnictogens. Angewandte Chemie, 2017, 129, 13606-13610.	1.6	6
89	Colossal Stability of Gas-Phase Trianions: Superpnictogens. Angewandte Chemie - International Edition, 2017, 56, 13421-13425.	7.2	23
90	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. Physical Review Letters, 2017, 119, 046403.	2.9	64

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91	Atomic-Level Design of Water-Resistant Hybrid Perovskites for Solar Cells by Using Cluster Ions. Journal of Physical Chemistry Letters, 2017, 8, 3726-3733.	2.1	15
92	Giant Valley Splitting and Valley Polarized Plasmonics in Group V Transition-Metal Dichalcogenide Monolayers. Journal of Physical Chemistry Letters, 2017, 8, 5764-5770.	2.1	19
93	Ī-Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry Letters, 2017, 8, 3234-3241.	2.1	205
94	Organozintl-based superatoms: [Ge ₉ (CHO) ₃] and [Ge ₉ (CHO)]. Chemical Physics Letters, 2017, 686, 195-202.	1.2	6
95	Substituent-Stabilized Organic Dianions in the Gas Phase and Their Potential Use as Electrolytes in Lithium-Ion Batteries. ChemPhysChem, 2016, 17, 2992-2997.	1.0	4
96	Stability of B ₁₂ (CN) ₁₂ ²⁺ : Implications for Lithium and Magnesium Ion Batteries. Angewandte Chemie, 2016, 128, 3768-3772.	1.6	28
97	Like Charges Attract?. Journal of Physical Chemistry Letters, 2016, 7, 2689-2695.	2.1	26
98	Stability of B ₁₂ (CN) ₁₂ ²⁺ : Implications for Lithium and Magnesium Ion Batteries. Angewandte Chemie - International Edition, 2016, 55, 3704-3708.	7.2	72
99	Integrating superconducting phase and topological crystalline quantum spin Hall effect in hafnium intercalated gallium film. Applied Physics Letters, 2016, 108, 253102.	1.5	4
100	Two-dimensional topological nanomaterials and related Hall effects. , 2016, , .		0
101	Many faces of carbon. Proceedings of SPIE, 2016, , .	0.8	1
102	Magnetic properties of bimetallic clusters composed of Gd and transition metals. Journal of Applied Physics, 2016, 119, 074301.	1.1	4
103	Changes in the photo-absorption spectrum of MEH-PPV in solution. , 2016, , .		0
104	Recent advances in 2D thermoelectric materials. Proceedings of SPIE, 2016, , .	0.8	4
105	Enhanced Carbon Dioxide Capture from Landfill Gas Using Bifunctionalized Benzimidazole-Linked Polymers. ACS Applied Materials & Interfaces, 2016, 8, 14648-14655.	4.0	76
106	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
107	Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. Journal of Physical Chemistry Letters, 2016, 7, 1919-1924.	2.1	33
108	Lattice thermal conductivity of penta-graphene. Carbon, 2016, 105, 424-429.	5.4	120

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109	Strain and carrier-induced coexistence of topologically insulating and superconducting phase in iodized Si(111) films. <i>Nano Research</i> , 2016, 9, 1578-1589.	5.8	6
110	Intrinsic quantum spin Hall and anomalous Hall effects in h-Sb/Bi epitaxial growth on a ferromagnetic MnO ₂ thin film. <i>Nanoscale</i> , 2016, 8, 11202-11209.	2.8	16
111	Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. <i>Physical Review B</i> , 2016, 94, .	1.1	7
112	Assembling π -Conjugated Molecules with Negative Gaussian Curvature for Efficient Carbon-Based Metal-Free Thermoelectric Material. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27829-27833.	1.5	7
113	Ferromagnetic and Half-Metallic FeC ₂ Monolayer Containing C ₂ Dimers. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 26207-26212.	4.0	58
114	Superhalogens as building blocks of two-dimensional organic-inorganic hybrid perovskites for optoelectronics applications. <i>Nanoscale</i> , 2016, 8, 17836-17842.	2.8	34
115	Pressure-induced structural transition in copper pyrazine dinitrate and implications for quantum magnetism. <i>Physical Review B</i> , 2016, 93, .	1.1	7
116	Complex metal borohydrides: multifunctional materials for energy storage and conversion. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 353001.	0.7	35
117	Investigation of hydrogen induced fluorescence in C ₆₀ and its potential use in luminescence down shifting applications. <i>Nanoscale</i> , 2016, 8, 18760-18770.	2.8	9
118	Assembling a bi-coordinated Cr complex for ferromagnetic nanorings: insight from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17868-17874.	1.3	0
119	Cluster-Inspired Design of High-Capacity Anode for Li-Ion Batteries. <i>ACS Energy Letters</i> , 2016, 1, 202-208.	8.8	23
120	SiTe monolayers: Si-based analogues of phosphorene. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6353-6361.	2.7	54
121	Structure and Properties of Egyptian Blue Monolayer Family: XCuSi ₄ O ₁₀ (X =) Tj ETQq1 1 0.784314,rgBT / 0	2.1	24
122	From Halogen to Superhalogen Behavior of Organic Molecules Created by Functionalizing Benzene. <i>ChemPhysChem</i> , 2016, 17, 184-189.	1.0	11
123	Organo-zintl Clusters [P ₇ R ₄]: A New Class of Superalkalis. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 800-805.	2.1	56
124	Super-ion inspired colorful hybrid perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 4728-4737.	5.2	84
125	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN ₂ Sheet. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3993-3998.	1.5	167
126	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8777-8784.	1.3	273

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127	High-temperature superconductivity in heavily N- or B-doped graphene. <i>Physical Review B</i> , 2015, 92, .	1.1	45
128	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. <i>Scientific Reports</i> , 2015, 5, 14342.	1.6	74
129	A novel strategy for reversible hydrogen storage in Ca(BH ₄) ₂ . <i>Chemical Communications</i> , 2015, 51, 11008-11011.	2.2	39
130	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17182-17189.	1.3	19
131	Electronic Structure and Stability of Mono- and Bimetallic Borohydrides and Their Underlying Hydrogen-Storage Properties: A Cluster Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11056-11061.	1.5	11
132	Mass spectrometry and its role in advancing cluster science. <i>International Journal of Mass Spectrometry</i> , 2015, 377, 235-247.	0.7	15
133	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 3689-3696.	3.8	22
134	Penta-graphene: A new carbon allotrope. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 2372-2377.	3.3	1,114
135	Structure and Properties of Polyfluoride F _n Clusters (n = 3-29). <i>Journal of Physical Chemistry A</i> , 2015, 119, 6483-6492.	1.1	13
136	Atomic Clusters: Opportunities in the Face of Challenges. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1549-1552.	2.1	17
137	Unusual stability of multiply charged organo-metallic complexes. <i>RSC Advances</i> , 2015, 5, 44003-44008.	1.7	16
138	Superhalogens: A Bridge between Complex Metal Hydrides and Li Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1119-1125.	2.1	38
139	Superhalogens beget superhalogens: a case study of (BO ₂) _n oligomers. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26589-26593.	1.3	11
140	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. <i>Nano Research</i> , 2015, 8, 2901-2912.	5.8	35
141	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24674-24680.	1.5	37
142	Tuning magnetic properties of antiferromagnetic chains by exchange interactions: ab initio studies. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26302-26306.	1.3	12
143	Catalytic activities of platinum nanotubes: a density functional study. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	2
144	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. <i>Nano Letters</i> , 2015, 15, 8277-8281.	4.5	168

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145	Self-assembly of metal atoms (Na, K, Ca) on graphene. <i>Nanoscale</i> , 2015, 7, 2352-2359.	2.8	10
146	Intermediate Phases during Decomposition of Metal Borohydrides, $M(\text{BH}_4)_n$ (M = Na, Mg, Y). <i>Journal of Physical Chemistry C</i> , 2014, 118, 28456-28461.	1.5	16
147	Tailoring Li adsorption on graphene. <i>Physical Review B</i> , 2014, 90, .	1.1	42
148	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd 13 cluster. <i>Physical Review B</i> , 2014, 89, .	1.1	26
149	Chain-like structures of gold supported by silicon substrate. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 924-932.	0.7	0
150	The viability of aluminum Zintl anion moieties within magnesium-aluminum clusters. <i>Journal of Chemical Physics</i> , 2014, 140, 124309.	1.2	35
151	Aluminum Zintl anion moieties within sodium aluminum clusters. <i>Journal of Chemical Physics</i> , 2014, 140, 054301.	1.2	37
152	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
153	Aromatic Superhalogens. <i>Chemistry - A European Journal</i> , 2014, 20, 4736-4745.	1.7	49
154	Anisotropic Mo ₂ Phthalocyanine Sheet: A New Member of the Organometallic Family. <i>Journal of Physical Chemistry A</i> , 2014, 118, 304-307.	1.1	13
155	Structures and Phase Transition of a MoS ₂ Monolayer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1515-1522.	1.5	432
156	Superalkalis and Superhalogens As Building Blocks of Supersalts. <i>Journal of Physical Chemistry A</i> , 2014, 118, 638-645.	1.1	119
157	Potential of ZrO clusters as replacement Pd catalyst. <i>Journal of Chemical Physics</i> , 2014, 141, 034301.	1.2	1
158	LiFe ₂ Cl _n (n = 4, 6) clusters: Double-exchange mediated molecular magnets. <i>Applied Physics Letters</i> , 2014, 105, 163112.	1.3	2
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