Puru Jena

List of Publications by Year in Descending Order

615 papers	25,827 citations	78 h-index	131 g-index
650 ext. papers	27,931 ext. citations	5.1 avg, IF	7.44 L-index

#	Paper	IF	Citations
615	SbCl: An Exceptional Superhalogen as the Building Block of a Mixed Valence Supercrystal with Unconventional Ferroelectricity.. *Journal of Physical Chemistry Letters*, **2022**, 1049-1056	6.4	0
614	Superatomic chemistry. *Journal of the Indian Chemical Society*, **2022**, 99, 100350		0
613	Halogen-Free Electrolytes Based on Modified Boranes for Alkali-Ion Batteries. *Journal of Physical Chemistry C*, **2022**, 126, 5112-5121	3.8	
612	Interfacial triferroicity in monolayer chromium dihalide. *Physical Review B*, **2022**, 105,	3.3	2
611	Review of modification strategies in emerging inorganic solid-state electrolytes for lithium, sodium, and potassium batteries. *Joule*, **2022**, 6, 543-587	27.8	8
610	Argyrodite-type advanced lithium conductors and transport mechanisms beyond peddle-wheel effect.. *Nature Communications*, **2022**, 13, 2078	17.4	3
609	Designing New Metal Chalcogenide Nanoclusters through Atom-by-Atom Substitution. *Small*, **2021**, 17, e2002927	11	3
608	Superatom-Based Ferroelectrics **2021**, 257-275		
607	Rational Design of Superatoms Using Electron-Counting Rules **2021**, 15-51		
606	Cluster-based Materials for Energy Harvesting and Storage **2021**, 277-316		
605	Clusters for CO 2 Activation and Conversion **2021**, 349-374		
604	Built-in electric field control of magnetic coupling in van der Waals semiconductors. *Physical Review B*, **2021**, 103,	3.3	4
603	Role of Size and Composition on the Design of Superalkalis. *Journal of Physical Chemistry A*, **2021**, 125, 5886-5894	2.8	2
602	Two-dimensional metal-free boron chalcogenides BX (X = Se and Te) as photocatalysts for water splitting under visible light. *Nanoscale*, **2021**, 13, 3627-3632	7.7	2
601	Imidazole-graphyne: a new 2D carbon nitride with a direct bandgap and strong IR refraction. *Physical Chemistry Chemical Physics*, **2021**, 23, 10274-10280	3.6	1
600	A family of ionic supersalts with covalent-like directionality and unconventional multiferroicity. *Nature Communications*, **2021**, 12, 1331	17.4	8
599	Binding of noble gas atoms by superhalogens. *Journal of Chemical Physics*, **2021**, 155, 014304	3.9	2

598	Antiperovskite KOI for K-Ion Solid State Electrolyte. *Journal of Physical Chemistry Letters*, **2021**, 12, 7120-7126	6.4	7
597	Theory-Guided Discovery of Novel Materials. *Journal of Physical Chemistry Letters*, **2021**, 12, 6499-6513	6.4	6
596	Heavily Tungsten-Doped Sodium Thioantimonate Solid-State Electrolytes with Exceptionally Low Activation Energy for Ionic Diffusion. *Angewandte Chemie - International Edition*, **2021**, 60, 26158-26166	16.4	7
595	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. *Carbon*, **2021**, 183, 652-659	10.4	3
594	Super-electrophiles of tri- and tetra-anions stabilized by selected terminal groups and their role in binding noble gas atoms. *Physical Chemistry Chemical Physics*, **2021**, 23, 21496-21500	3.6	2
593	Realization of the Zn oxidation state. *Nanoscale*, **2021**, 13, 14041-14048	7.7	1
592	Boron-Functionalized Organic Framework as a High-Performance Metal-Free Catalyst for N Fixation.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12142-12149	6.4	0
591	B2H6 splitting on catalytic surfaces and role of BH3 towards hydrogen spillover. *Journal of Power Sources*, **2020**, 455, 227973	8.9	0
590	A 3D porous honeycomb carbon as Na-ion battery anode material with high capacity, excellent rate performance, and robust stability. *Carbon*, **2020**, 168, 163-168	10.4	11
589	Robustness of Superatoms and Their Potential as Building Blocks of Materials: Al13⁻vs B(CN)4⁻ *Journal of Physical Chemistry C*, **2020**, 124, 6435-6440	3.8	6
588	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. *Physical Review Letters*, **2020**, 124, 067602	7.4	38
587	Clusters and Nanomaterials for Sustainable Energy. *ACS Energy Letters*, **2020**, 5, 428-429	20.1	1
586	Record-high stability and compactness of multiply-charged clusters aided by selected terminal groups. *Physical Chemistry Chemical Physics*, **2020**, 22, 4880-4883	3.6	6
585	Discovery of twin orbital-order phases in ferromagnetic semiconducting VI monolayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 512-517	3.6	18
584	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. *Journal of Power Sources*, **2020**, 478, 228746	8.9	7
583	Assembling SiBN nanoribbons into a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance. *Nanoscale*, **2020**, 12, 19367-19374	7.7	8
582	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. *Journal of Physical Chemistry Letters*, **2020**, 11, 3501-3506	6.4	31
581	Yttrium-Sodium Halides as Promising Solid-State Electrolytes with High Ionic Conductivity and Stability for Na-Ion Batteries. *Journal of Physical Chemistry Letters*, **2020**, 11, 3376-3383	6.4	16

580	Rational Design of Porous Nodal-Line Semimetallic Carbon for K-Ion Battery Anode Materials. *Journal of Physical Chemistry Letters*, **2019**, 10, 6360-6367	6.4	21
579	Boronated holey graphene: a case of 2D ferromagnetic metal. *Physical Chemistry Chemical Physics*, **2019**, 21, 21128-21135	3.6	2
578	Ligand stabilization of manganocene dianions - in defiance of the 18-electron rule. *Physical Chemistry Chemical Physics*, **2019**, 21, 24300-24307	3.6	5
577	Homocoupling and Heterocoupling of Grignard Perfluorobenzene Reagents via Aryne Intermediates: A DFT Study. *Journal of Physical Chemistry A*, **2019**, 123, 9693-9700	2.8	0
576	Conserved Vibrational Coherence in the Ultrafast Rearrangement of 2-Nitrotoluene Radical Cation. *Journal of Physical Chemistry A*, **2019**, 123, 1140-1152	2.8	16
575	A high-pressure induced stable phase of Li2MnSiO4 as an effective poly-anion cathode material from simulations. *Journal of Materials Chemistry A*, **2019**, 7, 16406-16413	13	5
574	Tuning range-separated DFT functionals for modeling the peak absorption of MEH-PPV polymer in various solvents. *Computational and Theoretical Chemistry*, **2019**, 1162, 112506	2	3
573	Stable Tetra- and Penta-Anions in the Gas Phase. *Angewandte Chemie - International Edition*, **2019**, 58, 11248-11252	16.4	12
572	N-doped peanut-shaped carbon nanotubes for efficient CO2 electrocatalytic reduction. *Carbon*, **2019**, 152, 241-246	10.4	17
571	Rational Design of Stable Dianions and the Concept of Super-Chalcogens. *Journal of Physical Chemistry A*, **2019**, 123, 5753-5761	2.8	5
570	Superhalogens as Building Blocks of Super Lewis Acids. *ChemPhysChem*, **2019**, 20, 1607-1612	3.2	9
569	Mechanistic Insight into Photocatalytic Pathways of MIL-100(Fe)/TiO Composites. *ACS Applied Materials & Interfaces*, **2019**, 11, 12516-12524	9.5	54
568	Tetragonal C24: a topological nodal-surface semimetal with potential as an anode material for sodium ion batteries. *Journal of Materials Chemistry A*, **2019**, 7, 5733-5739	13	40
567	Unique reactivity of B in B[GeY] (Y = H, CH, BO, CN): formation of a Lewis base. *Physical Chemistry Chemical Physics*, **2019**, 21, 23301-23304	3.6	3
566	Hydrogenated C60 as High-Capacity Stable Anode Materials for Li Ion Batteries. *ACS Applied Energy Materials*, **2019**, 2, 6453-6460	6.1	14
565	Lattice Dynamic and Instability in Pentasilicene: A Light Single-Element Ferroelectric Material With High Curie Temperature. *Physical Review Applied*, **2019**, 11,	4.3	14
564	Stable Tetra- and Penta-Anions in the Gas Phase. *Angewandte Chemie*, **2019**, 131, 11370-11374	3.6	
563	Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI3 Monolayer through van der Waals Heterostructures. *Journal of Physical Chemistry C*, **2019**, 123, 17987-17993	3.8	38

562	Interfacial properties of penta-graphene-metal contacts. *Journal of Applied Physics*, **2019**, 125, 065308	2.5	6
561	Innentitelbild: Stable Tetra- and Penta-Anions in the Gas Phase (Angew. Chem. 33/2019). *Angewandte Chemie*, **2019**, 131, 11246	3.6	
560	Sodium Superionic Conductors Based on Clusters. *ACS Applied Materials & Interfaces*, **2019**, 11, 963-972	9.5	29
559	Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters. *Journal of Physical Chemistry A*, **2018**, 122, 4350-4356	2.8	4
558	Dissociation dynamics of 3- and 4-nitrotoluene radical cations: Coherently driven C-NO bond homolysis. *Journal of Chemical Physics*, **2018**, 148, 134305	3.9	13
557	A metallic peanut-shaped carbon nanotube and its potential for CO2 capture. *Carbon*, **2018**, 132, 249-256	10.4	7
556	Ultrafast coherent vibrational dynamics in dimethyl methylphosphonate radical cation. *Physical Chemistry Chemical Physics*, **2018**, 20, 4636-4640	3.6	10
555	Effect of hydrogenation on the structure and magnetic properties of an iron oxide cluster. *Physical Chemistry Chemical Physics*, **2018**, 20, 4546-4553	3.6	8
554	Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metal□Organic Coordination Networks. *Advanced Electronic Materials*, **2018**, 4, 1700323	6.4	10
553	The rise of two-dimensional van der Waals ferroelectrics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1365	7.9	89
552	Co-mixing hydrogen and methane may double the energy storage capacity. *Journal of Materials Chemistry A*, **2018**, 6, 8916-8922	13	11
551	Simultaneous Detection and Removal of Formaldehyde at Room Temperature: Janus Au@ZnO@ZIF-8 Nanoparticles. *Nano-Micro Letters*, **2018**, 10, 4	19.5	55
550	Electron affinity of modified benzene. *International Journal of Quantum Chemistry*, **2018**, 118, e25504	2.1	13
549	Discovery of a high-pressure phase of rutile-like CoO2 and its potential as a cathode material. *Journal of Materials Chemistry A*, **2018**, 6, 18449-18457	13	4
548	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	13	31
547	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. *Physical Review Materials*, **2018**, 2,	3.2	13
546	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. *Carbon*, **2018**, 127, 527-532	10.4	28
545	B(SCN)4□A New Weakly Coordinating Anion in the Tetracyanoborate Family. *Journal of Physical Chemistry C*, **2018**, 122, 13371-13375	3.8	5

544	Super-alkalis as building blocks of one-dimensional hierarchical electrides. *Nanoscale*, **2018**, 10, 22963-22969	7.7	10
543	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. *Chemical Reviews*, **2018**, 118, 5755-5870	68.1	265
542	Collective Superexchange and Exchange Coupling Constants in the Hydrogenated Iron Oxide Particle FeOH. *Journal of Physical Chemistry A*, **2018**, 122, 5043-5049	2.8	1
541	Body-Centered Tetragonal C : A Novel Topological Node-Line Semimetallic Carbon Composed of Tetrarings. *Small*, **2017**, 13, 1602894	11	49
540	Two-dimensional topological crystalline quantum spin Hall effect in transition metal intercalated compounds. *Physical Review B*, **2017**, 95,	3.3	8
539	Rational design of super-alkalis and their role in CO activation. *Nanoscale*, **2017**, 9, 4891-4897	7.7	47
538	Superhalogen-based lithium superionic conductors. *Journal of Materials Chemistry A*, **2017**, 5, 13373-13381	8	40
537	Rational Design of Stable Dianions by Functionalizing Polycyclic Aromatic Hydrocarbons. *ChemPhysChem*, **2017**, 18, 1937-1942	3.2	3
536	Role of ligands in the stability of BX and CBX (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	3.6	17
535	B12(SCN)12□An Ultrastable Weakly Coordinating Dianion. *Journal of Physical Chemistry C*, **2017**, 121, 7697-7702	3.8	24
534	Quantum anomalous Hall effect in ferromagnetic transition metal halides. *Physical Review B*, **2017**, 95,	3.3	69
533	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	2.8	14
532	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	11.5	76
531	Exceptional Thermoelectric Properties of Layered GeAs2. *Chemistry of Materials*, **2017**, 29, 9300-9307	9.6	47
530	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie*, **2017**, 129, 13606-13610	3.6	6
529	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie - International Edition*, **2017**, 56, 13421-13425	16.4	15
528	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. *Physical Review Letters*, **2017**, 119, 046403	7.4	22
527	Atomic-Level Design of Water-Resistant Hybrid Perovskites for Solar Cells by Using Cluster Ions. *Journal of Physical Chemistry Letters*, **2017**, 8, 3726-3733	6.4	10

526	Giant Valley Splitting and Valley Polarized Plasmonics in Group V Transition-Metal Dichalcogenide Monolayers. *Journal of Physical Chemistry Letters*, **2017**, 8, 5764-5770	6.4	17
525	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	6.4	109
524	Organo Zintl-based superatoms: [Ge9(CHO)3] and [Ge9(CHO)]. *Chemical Physics Letters*, **2017**, 686, 195-202	2.5	5
523	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. *Physical Chemistry Chemical Physics*, **2016**, 18, 8777-84	3.6	198
522	Assembling Conjugated Molecules with Negative Gaussian Curvature for Efficient Carbon-Based Metal-Free Thermoelectric Material. *Journal of Physical Chemistry C*, **2016**, 120, 27829-27833	3.8	4
521	Ferromagnetic and Half-Metallic FeC Monolayer Containing C Dimers. *ACS Applied Materials & Interfaces*, **2016**, 8, 26207-26212	9.5	44
520	Superhalogens as building blocks of two-dimensional organic-inorganic hybrid perovskites for optoelectronics applications. *Nanoscale*, **2016**, 8, 17836-17842	7.7	32
519	Pressure-induced structural transition in copper pyrazine dinitrate and implications for quantum magnetism. *Physical Review B*, **2016**, 93,	3.3	5
518	Complex metal borohydrides: multifunctional materials for energy storage and conversion. *Journal of Physics Condensed Matter*, **2016**, 28, 353001	1.8	27
517	Investigation of hydrogen induced fluorescence in C and its potential use in luminescence down shifting applications. *Nanoscale*, **2016**, 8, 18760-18770	7.7	9
516	Assembling a bi-coordinated Cr complex for ferromagnetic nanorings: insight from first-principles calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 17868-74	3.6	
515	Cluster-Inspired Design of High-Capacity Anode for Li-Ion Batteries. *ACS Energy Letters*, **2016**, 1, 202-208	20.1	19
514	SiTe monolayers: Si-based analogues of phosphorene. *Journal of Materials Chemistry C*, **2016**, 4, 6353-6361	7.1	44
513	Structure and Properties of Egyptian Blue Monolayer Family: XCuSi4O10 (X = Ca, Sr, and Ba). *Journal of Physical Chemistry Letters*, **2016**, 7, 399-405	6.4	16
512	From Halogen to Superhalogen Behavior of Organic Molecules Created by Functionalizing Benzene. *ChemPhysChem*, **2016**, 17, 184-9	3.2	10
511	Organo-Zintl Clusters [P7R4]: A New Class of Superalkalis. *Journal of Physical Chemistry Letters*, **2016**, 7, 800-5	6.4	41
510	Super-ion inspired colorful hybrid perovskite solar cells. *Journal of Materials Chemistry A*, **2016**, 4, 4728-4737	10	74
509	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN2 Sheet. *Journal of Physical Chemistry C*, **2016**, 120, 3993-3998	3.8	125

508	Substituent-Stabilized Organic Dianions in the Gas Phase and Their Potential Use as Electrolytes in Lithium-Ion Batteries. *ChemPhysChem*, **2016**, 17, 2992-2997	3.2	3
507	Stability of B12(CN)122Implications for Lithium and Magnesium Ion Batteries. *Angewandte Chemie*, **2016**, 128, 3768-3772	3.6	19
506	Like Charges Attract?. *Journal of Physical Chemistry Letters*, **2016**, 7, 2689-95	6.4	23
505	Stability of B12 (CN)12 (2-) : Implications for Lithium and Magnesium Ion Batteries. *Angewandte Chemie - International Edition*, **2016**, 55, 3704-8	16.4	57
504	Integrating superconducting phase and topological crystalline quantum spin Hall effect in hafnium intercalated gallium film. *Applied Physics Letters*, **2016**, 108, 253102	3.4	4
503	Many faces of carbon **2016**,		1
502	Magnetic properties of bimetallic clusters composed of Gd and transition metals. *Journal of Applied Physics*, **2016**, 119, 074301	2.5	4
501	Recent advances in 2D thermoelectric materials **2016**,		4
500	Enhanced Carbon Dioxide Capture from Landfill Gas Using Bifunctionalized Benzimidazole-Linked Polymers. *ACS Applied Materials & Interfaces*, **2016**, 8, 14648-55	9.5	64
499	Molecular Origin of Properties of Organic-Inorganic Hybrid Perovskites: The Big Picture from Small Clusters. *Journal of Physical Chemistry Letters*, **2016**, 7, 1596-603	6.4	50
498	Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. *Journal of Physical Chemistry Letters*, **2016**, 7, 1919-24	6.4	26
497	Lattice thermal conductivity of penta-graphene. *Carbon*, **2016**, 105, 424-429	10.4	77
496	Strain and carrier-induced coexistence of topologically insulating and superconducting phase in iodized Si(111) films. *Nano Research*, **2016**, 9, 1578-1589	10	5
495	Intrinsic quantum spin Hall and anomalous Hall effects in h-Sb/Bi epitaxial growth on a ferromagnetic MnO2 thin film. *Nanoscale*, **2016**, 8, 11202-9	7.7	12
494	Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. *Physical Review B*, **2016**, 94,	3.3	5
493	Structure and Properties of Polyfluoride Fn(-) Clusters (n = 3-29). *Journal of Physical Chemistry A*, **2015**, 119, 6483-92	2.8	12
492	Atomic Clusters: Opportunities in the Face of Challenges. *Journal of Physical Chemistry Letters*, **2015**, 6, 1549-52	6.4	15
491	Unusual stability of multiply charged organo-metallic complexes. *RSC Advances*, **2015**, 5, 44003-44008	3.7	14

490	Superhalogens: A Bridge between Complex Metal Hydrides and Li Ion Batteries. *Journal of Physical Chemistry Letters*, **2015**, 6, 1119-25	6.4	31
489	Superhalogens beget superhalogens: a case study of (BO2)n oligomers. *Physical Chemistry Chemical Physics*, **2015**, 17, 26589-93	3.6	10
488	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. *Nano Research* , **2015**, 8, 2901-2912	10	28
487	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. *Journal of Physical Chemistry C*, **2015**, 119, 24674-24680	3.8	32
486	Tuning magnetic properties of antiferromagnetic chains by exchange interactions: ab initio studies. *Physical Chemistry Chemical Physics*, **2015**, 17, 26302-6	3.6	11
485	Catalytic activities of platinum nanotubes: a density functional study. *European Physical Journal B*, **2015**, 88, 1	1.2	2
484	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. *Nano Letters*, **2015**, 15, 8277-81	11.5	132
483	Self-assembly of metal atoms (Na, K, Ca) on graphene. *Nanoscale*, **2015**, 7, 2352-9	7.7	10
482	High-temperature superconductivity in heavily N- or B-doped graphene. *Physical Review B*, **2015**, 92,	3.3	33
481	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. *Scientific Reports*, **2015**, 5, 14342	4.9	62
480	A novel strategy for reversible hydrogen storage in Ca(BH4)2. *Chemical Communications*, **2015**, 51, 11008-11	5.8	37
479	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. *Physical Chemistry Chemical Physics*, **2015**, 17, 17182-9	3.6	15
478	Electronic Structure and Stability of Mono- and Bimetallic Borohydrides and Their Underlying Hydrogen-Storage Properties: A Cluster Study. *Journal of Physical Chemistry C*, **2015**, 119, 11056-11061	3.8	11
477	Mass spectrometry and its role in advancing cluster science. *International Journal of Mass Spectrometry*, **2015**, 377, 235-247	1.9	13
476	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. *International Journal of Hydrogen Energy*, **2015**, 40, 3689-3696	6.7	17
475	Penta-graphene: A new carbon allotrope. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 2372-7	11.5	763
474	Pressure-induced magnetic crossover driven by hydrogen bonding in CuF(HF)(3-chloropyridine). *Scientific Reports*, **2014**, 4, 6054	4.9	18
473	Aromatic superhalogens. *Chemistry - A European Journal*, **2014**, 20, 4736-45	4.8	38

472	Anisotropic Mo2-phthalocyanine sheet: a new member of the organometallic family. *Journal of Physical Chemistry A*, **2014**, 118, 304-7	2.8	7
471	Structures and Phase Transition of a MoS2 Monolayer. *Journal of Physical Chemistry C*, **2014**, 118, 1515-1522	4.8	356
470	Superalkalis and superhalogens as building blocks of supersalts. *Journal of Physical Chemistry A*, **2014**, 118, 638-45	2.8	98
469	Potential of ZrO clusters as replacement Pd catalyst. *Journal of Chemical Physics*, **2014**, 141, 034301	3.9	1
468	LiFe2Cln (n = 4-8) clusters: Double-exchange mediated molecular magnets. *Applied Physics Letters*, **2014**, 105, 163112	3.4	2
467	Identification of hyperhalogens in Ag(n)(BO2)(m) (n = 1-3, m = 1-2) clusters: anion photoelectron spectroscopy and density functional calculations. *Physical Chemistry Chemical Physics*, **2014**, 16, 26067-74	3.6	11
466	New insights into carbon dioxide interactions with benzimidazole-linked polymers. *Chemical Communications*, **2014**, 50, 3571-4	5.8	43
465	Organic superhalogens. *ChemPhysChem*, **2014**, 15, 2903-8	3.2	23
464	Superhalogens as building blocks of halogen-free electrolytes in lithium-ion batteries. *Angewandte Chemie - International Edition*, **2014**, 53, 13916-9	16.4	93
463	Tuning electronic and magnetic properties of silicene with magnetic superhalogens. *Physical Chemistry Chemical Physics*, **2014**, 16, 22979-86	3.6	30
462	Alanate anion, AlH4(-): photoelectron spectrum and computations. *Journal of Physical Chemistry A*, **2014**, 118, 8158-62	2.8	19
461	Structural, electronic and magnetic properties of neutral and anionic Fe2(BO2)n (n=1-3) clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2959-2964	2.3	3
460	18-Electron rule inspired Zintl-like ions composed of all transition metals. *Physical Chemistry Chemical Physics*, **2014**, 16, 20241-7	3.6	7
459	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. *Nanoscale*, **2014**, 6, 14962-70	7.7	25
458	Origin of Red Shift in the Photoabsorption Peak in MEH-PPV Polymer. *Journal of Physical Chemistry C*, **2014**, 118, 13444-13450	3.8	11
457	Receptor-ligand interaction at 5-HT3 serotonin receptors: a cluster approach. *Journal of Physical Chemistry A*, **2014**, 118, 8471-6	2.8	2
456	Superhalogens as Building Blocks of Halogen-Free Electrolytes in Lithium-Ion Batteries. *Angewandte Chemie*, **2014**, 126, 14136-14139	3.6	26
455	Intermediate Phases during Decomposition of Metal Borohydrides, M(BH4)n (M = Na, Mg, Y). *Journal of Physical Chemistry C*, **2014**, 118, 28456-28461	3.8	15

454	Tailoring Li adsorption on graphene. *Physical Review B*, **2014**, 90,	3.3	36
453	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd13 cluster. *Physical Review B*, **2014**, 89,	3.3	20
452	Chain-like structures of gold supported by silicon substrate. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 924-932	1.3	
451	The viability of aluminum Zintl anion moieties within magnesium-aluminum clusters. *Journal of Chemical Physics*, **2014**, 140, 124309	3.9	35
450	Aluminum Zintl anion moieties within sodium aluminum clusters. *Journal of Chemical Physics*, **2014**, 140, 054301	3.9	34
449	Lithium-doped triazine-based graphitic C3N4 sheet for hydrogen storage at ambient temperature. *Computational Materials Science*, **2014**, 81, 275-279	3.2	53
448	Magnetic hollow cages with colossal moments. *Journal of Chemical Physics*, **2013**, 139, 044301	3.9	6
447	Unusual Magnetic Properties of Functionalized Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2013**, 4, 2482-2488	6.4	22
446	Competition between surface chemisorption and cage formation in Fe12O12 clusters. *Chemical Physics Letters*, **2013**, 556, 211-216	2.5	22
445	Stable three-dimensional metallic carbon with interlocking hexagons. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 18809-13	11.5	100
444	Structure and properties of Mn4Cl9: an antiferromagnetic binary hyperhalogen. *Journal of Chemical Physics*, **2013**, 138, 054309	3.9	41
443	Three-dimensional metallic boron nitride. *Journal of the American Chemical Society*, **2013**, 135, 18216-21	16.4	113
442	Synthesis, Characterization, and Atomistic Modeling of Stabilized Highly Pyrophoric Al(BH4)3 via the Formation of the Hypersalt K[Al(BH4)4]. *Journal of Physical Chemistry C*, **2013**, 117, 19905-19915	3.8	44
441	The Intrinsic Ferromagnetism in a MnO2 Monolayer. *Journal of Physical Chemistry Letters*, **2013**, 4, 3382-6	6.4	142
440	Electronic and magnetic properties of pristine and transition metal doped ZnTe nanowires. *Journal of Physics Condensed Matter*, **2013**, 25, 266003	1.8	2
439	All-metal clusters that mimic the chemistry of halogens. *ChemPhysChem*, **2013**, 14, 3227-32	3.2	8
438	Role of Ti-based catalysts in the dehydrogenation mechanism of magnesium borohydride: A cluster approach. *International Journal of Hydrogen Energy*, **2013**, 38, 2357-2362	6.7	13
437	Structure, stability and superhalogen properties of sodium and magnesium borohydrides. *Chemical Physics Letters*, **2013**, 556, 173-177	2.5	18

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