Puru Jena

List of Publications by Citations

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	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
614	Ferromagnetism in semihydrogenated graphene sheet. *Nano Letters*, **2009**, 9, 3867-70	11.5	686
613	Materials for Hydrogen Storage: Past, Present, and Future. *Journal of Physical Chemistry Letters*, **2011**, 2, 206-211	6.4	676
612	Clustering of Ti on a C60 surface and its effect on hydrogen storage. *Journal of the American Chemical Society*, **2005**, 127, 14582-3	16.4	606
611	Assembling crystals from clusters. *Physical Review Letters*, **1992**, 69, 1664-1667	7.4	504
610	First-principles study of hydrogen storage on Li12C60. *Journal of the American Chemical Society*, **2006**, 128, 9741-5	16.4	474
609	Hydrogen interactions with defects in crystalline solids. *Reviews of Modern Physics*, **1992**, 64, 559-617	40.5	417
608	Vacancy-induced magnetism in ZnO thin films and nanowires. *Physical Review B*, **2008**, 77,	3.3	381
607	Atomic clusters: Building blocks for a class of solids. *Physical Review B*, **1995**, 51, 13705-13716	3.3	367
606	Structures and Phase Transition of a MoS2 Monolayer. *Journal of Physical Chemistry C*, **2014**, 118, 1515-1522	4.8	356
605	Evolution of the electronic structure and properties of neutral and charged aluminum clusters: A comprehensive analysis. *Journal of Chemical Physics*, **1999**, 111, 1890-1904	3.9	314
604	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. *Chemical Reviews*, **2018**, 118, 5755-5870	68.1	265
603	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. *Physical Review B*, **2010**, 81,	3.3	247
602	Magic numbers in metallo-inorganic clusters: chromium encapsulated in silicon cages. *Physical Review Letters*, **2002**, 89, 016803	7.4	227
601	Beyond the Periodic Table of Elements: The Role of Superatoms. *Journal of Physical Chemistry Letters*, **2013**, 4, 1432-42	6.4	207
600	Electronic structure and properties of transition metal-benzene complexes. *Journal of the American Chemical Society*, **2001**, 123, 3799-808	16.4	207
599	Clusters: a bridge across the disciplines of physics and chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 10560-9	11.5	201

598	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. *Physical Chemistry Chemical Physics*, **2016**, 18, 8777-84	3.6	198
597	Direct observation of key reaction intermediates on gold clusters. *Journal of the American Chemical Society*, **2003**, 125, 2848-9	16.4	196
596	Electric field enhanced hydrogen storage on polarizable materials substrates. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 2801-6	11.5	194
595	Binding of hydrogen molecules by a transition-metal ion. *Physical Review Letters*, **1992**, 68, 2277-2280	7.4	191
594	Potential of AlN nanostructures as hydrogen storage materials. *ACS Nano*, **2009**, 3, 621-6	16.7	183
593	Carbon nanomaterials as catalysts for hydrogen uptake and release in NaAlH4. *Nano Letters*, **2009**, 9, 1501-5	11.5	180
592	Electronic structures and bonding of graphyne sheet and its BN analog. *Journal of Chemical Physics*, **2011**, 134, 174701	3.9	163
591	Unexpected stability of Al4H6: a borane analog?. *Science*, **2007**, 315, 356-8	33.3	155
590	Physics of small metal clusters: Topology, magnetism, and electronic structure. *Physical Review B*, **1985**, 32, 2058-2069	3.3	152
589	Spin conservation accounts for aluminum cluster anion reactivity pattern with O2. *Science*, **2008**, 319, 438-42	33.3	147
588	The Intrinsic Ferromagnetism in a MnO2 Monolayer. *Journal of Physical Chemistry Letters*, **2013**, 4, 3382-6	6.4	142
587	Giant magnetic moments of nitrogen-doped Mn clusters and their relevance to ferromagnetism in Mn-doped GaN. *Physical Review Letters*, **2002**, 89, 185504	7.4	138
586	Systematic Study of Oxo, Peroxo, and Superoxo Isomers of 3d-Metal Dioxides and Their Anions. *Journal of Physical Chemistry A*, **2000**, 104, 11961-11971	2.8	138
585	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. *Nano Letters*, **2015**, 15, 8277-81	11.5	132
584	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. *Journal of Physical Chemistry C* , **2013**, 117, 6055-6059	3.8	131
583	Hyperhalogens: discovery of a new class of highly electronegative species. *Angewandte Chemie - International Edition*, **2010**, 49, 8966-70	16.4	131
582	Hydrogen storage and the 18-electron rule. *Journal of Chemical Physics*, **2006**, 124, 224703	3.9	128
581	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN2 Sheet. *Journal of Physical Chemistry C*, **2016**, 120, 3993-3998	3.8	125

580	Origin of the unusual stability of MnO4. *Chemical Physics Letters*, **1999**, 312, 598-605	2.5	125
579	Geometry and electronic structure of Vn(Bz)m complexes. *Journal of Chemical Physics*, **2004**, 120, 10414-22	3.9	124
578	Magnetism and local order: Ab initio tight-binding theory. *Physical Review B*, **1989**, 39, 6914-6924	3.3	119
577	Electronic structure and magnetism of Rhn (n=2-13) clusters. *Physical Review B*, **1999**, 59, 5214-5222	3.3	117
576	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. *Journal of Chemical Theory and Computation*, **2009**, 5, 374-9	6.4	115
575	Three-dimensional metallic boron nitride. *Journal of the American Chemical Society*, **2013**, 135, 18216-21	16.4	113
574	Structure and bonding of Au5M (M=Na, Mg, Al, Si, P, and S) clusters. *Physical Review B*, **2006**, 74,	3.3	110
573	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
572	Carrier-mediated ferromagnetism in N codoped (Zn,Mn)O (10-10) thin films. *Physical Review B*, **2004**, 70,	3.3	109
571	Atomic and electronic structure of neutral and charged SinOm clusters. *Journal of Chemical Physics*, **1998**, 109, 1245-1250	3.9	108
570	Anomalous magnetism in small Mn clusters. *Chemical Physics Letters*, **1998**, 289, 473-479	2.5	106
569	Optical properties of Ti3SiC2 and Ti4AlN3. *Applied Physics Letters*, **2008**, 92, 221907	3.4	106
568	Magnetism in small vanadium clusters. *Physical Review B*, **1991**, 43, 8179-8182	3.3	106
567	Physics of Nickel Clusters. 2. Electronic Structure and Magnetic Properties. *Journal of Physical Chemistry A*, **1998**, 102, 1748-1759	2.8	105
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565	Electronic structure of chromium oxides, CrOn and CrOn (n=1-5) from photoelectron spectroscopy and density functional theory calculations. *Journal of Chemical Physics*, **2001**, 115, 7935-7944	3.9	105
564	Temperature Dependence of Electric Field Gradients in Noncubic Metals. *Physical Review Letters*, **1976**, 36, 418-421	7.4	104
563	Interactions of Au cluster anions with oxygen. *Journal of Chemical Physics*, **2004**, 120, 6510-5	3.9	101

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561	Electronic structure of hydrogen in simple metals. *Physical Review B*, **1978**, 17, 3518-3524	3.3	99
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559	Unique magnetic signature of transition metal atoms supported on benzene. *Chemical Physics Letters*, **2000**, 321, 142-150	2.5	97
558	Physics of Nickel Clusters: Energetics and Equilibrium Geometries. *Journal of Physical Chemistry A*, **1997**, 101, 1072-1080	2.8	96
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556	Electronic, magnetic, and geometric structure of metallo-carbohedrenes. *Science*, **1992**, 258, 1640-3	33.3	95
555	Electronic Structure of the 3d Metal Monoxide Anions. *Journal of Physical Chemistry A*, **2000**, 104, 5374-5379	2.8	94
554	Superhalogens as building blocks of halogen-free electrolytes in lithium-ion batteries. *Angewandte Chemie - International Edition*, **2014**, 53, 13916-9	16.4	93
553	Atomic and electronic structures of neutral and charged boron and boron-rich clusters. *Journal of Chemical Physics*, **1997**, 107, 132-140	3.9	92
552	The rise of two-dimensional van der Waals ferroelectrics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1365	7.9	89
551	Ferromagnetism in Mn-doped GaN nanowires. *Physical Review Letters*, **2005**, 95, 167202	7.4	89
550	Electronic signature of the magicity and ionic bonding in Al13X (X=Li) clusters. *Physical Review B*, **2002**, 65,	3.3	89
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548	Ferromagnetism in small clusters. *Physical Review Letters*, **1991**, 66, 938-941	7.4	84
547	Closo-alanes (Al4H4, AlnHn+2, 4 . *Journal of the American Chemical Society*, **2007**, 129, 5969-75	16.4	83
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545	Functionalized heterofullerenes for hydrogen storage. *Applied Physics Letters*, **2009**, 94, 013111	3.4	82

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542	Equilibrium Geometry, Stability, and Magnetic Properties of Small MnO Clusters. *Journal of the American Chemical Society*, **1999**, 121, 644-652	16.4	81
541	Highly selective CO2/CH4 gas uptake by a halogen-decorated borazine-linked polymer. *Journal of Materials Chemistry*, **2012**, 22, 13524		80
540	Magnetic properties of transition-metal-doped Zn1−xTxO (T=Cr, Mn, Fe, Co, and Ni) thin films with and without intrinsic defects: A density functional study. *Physical Review B*, **2009**, 79,	3.3	79
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534	Hydroxyl-decorated graphene systems as candidates for organic metal-free ferroelectrics, multiferroics, and high-performance proton battery cathode materials. *Physical Review B*, **2013**, 87,	3.3	77
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532	Lattice thermal conductivity of penta-graphene. *Carbon*, **2016**, 105, 424-429	10.4	77
531	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
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