

Swapan K Pati

List of Publications by Year in descending order

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264
papers

10,547
citations

34016

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269
docs citations

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times ranked

13825
citing authors

#	ARTICLE	IF	CITATIONS
1	Novel design of single transition metal atoms anchored on C ₆ N ₆ nanosheet for electrochemical and photochemical N ₂ reduction to Ammonia. <i>Catalysis Today</i> , 2023, 424, 113804.	2.2	6
2	Loss of classicality in alternating spin-1/2 /spin-1 chain, in the presence of next-neighbor couplings and Dzyaloshinskiiâ€“Moriya interactions. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 175802.	0.7	0
3	Chiral Arylene Diimide Phosphors: Circularly Polarized Ambient Phosphorescence from Bischromophoric Pyromellitic Diimides. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	33
4	Polaronic Signatures in Doped and Undoped Cesium Lead Halide Perovskite Nanocrystals through a Photoinduced Raman Mode. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 5567-5577.	4.0	1
5	Activation of O ₂ across a C(sp ³)â€“C(sp ³) bond. <i>Chemical Communications</i> , 2022, 58, 3122-3125.	2.2	0
6	Potassium Cobalt Pyrophosphate as a Nonprecious Bifunctional Electrocatalyst for Zincâ€“Air Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 8992-9001.	4.0	9
7	Impacts of CsPbBr ₃ /PbSe Heterostructures on Carrier Cooling Dynamics at Low Carrier Density. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	16
8	Influence of Noncovalent Interactions on the Magnetic Behavior of Three Isostructural Layered Manganese(II) Dicarboxylate-Based Coordination Polymers. <i>Crystal Growth and Design</i> , 2022, 22, 2534-2546.	1.4	6
9	Computational Insight into TMâ€“N Embedded Graphene Bifunctional Electrocatalysts for Oxygen Evolution and Reduction Reactions. <i>ACS Physical Chemistry Au</i> , 2022, 2, 305-315.	1.9	10
10	Recent Advances in Group 14 and 15 Lewis Acids for Frustrated Lewis Pair Chemistry. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	9
11	Anchoring boron on a covalent organic framework as an efficient single atom metal-free photo-electrocatalyst for nitrogen fixation: a first-principles analysis. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10765-10774.	1.3	12
12	3dâ€“Transition metal doped two-dimensional SnTe: Modulation of thermoelectric properties. <i>Materials Today Communications</i> , 2022, 31, 103656.	0.9	2
13	Anionâ€“Induced Room Temperature Phosphorescence from Emissive Charge-Transfer States. <i>Journal of the American Chemical Society</i> , 2022, 144, 10854-10861.	6.6	46
14	Modulating the Carrier Relaxation Dynamics in Heterovalently (Bi ³⁺) Doped CsPbBr ₃ Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5431-5440.	2.1	18
15	Unraveling the formation mechanism of NaCoPO ₄ polymorphs. <i>Journal of Solid State Chemistry</i> , 2021, 293, 121766.	1.4	4
16	Effect of conjugation on the vibrational modes of a carbon nanotube dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118985.	2.0	4
17	Bicyclic (alkyl)(amino)carbene stabilized zinc(0) complex with singlet biradicaloid ground state. <i>Chemical Communications</i> , 2021, 57, 5282-5285.	2.2	14
18	A small heterocyclic molecule as a multistate transistor: a quantum many-body approach. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10927-10934.	2.7	2

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19	Computational Exploration of Intramolecular Sn/N Frustrated Lewis Pairs for Hydrogen Activation and Catalytic Hydrogenation. <i>Organometallics</i> , 2021, 40, 194-202.	1.1	8
20	Exploring a Superlattice of SnO-PbO: A New Material for Thermoelectric Applications. <i>ACS Applied Energy Materials</i> , 2021, 4, 2081-2090.	2.5	7
21	In Situ Cation Intercalation in the Interlayer of Tungsten Sulfide with Overlaying Layered Double Hydroxide in a 2D Heterostructure for Facile Electrochemical Redox Activity. <i>Inorganic Chemistry</i> , 2021, 60, 6911-6921.	1.9	17
22	Ambient Room Temperature Phosphorescence and Thermally Activated Delayed Fluorescence from a Core-Substituted Pyromellitic Diimide Derivative. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4520-4526.	1.2	21
23	Arylene Diimide Phosphors: Aggregation Modulated Twin Room Temperature Phosphorescence from Pyromellitic Diimides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 12323-12327.	7.2	93
24	Light Harvesting Supramolecular Phosphors: Highly Efficient Room Temperature Phosphorescence in Solution and Hydrogels. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19720-19724.	7.2	135
25	Intersystem Crossing in Boron-Based Donor-Spiro-Acceptor Organic Chromophore: A Detailed Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6674-6680.	1.1	15
26	Achievement of strain-driven ultrahigh carrier mobility in $\text{In}_2\text{-TeO}_2$. <i>Materials Research Bulletin</i> , 2021, 141, 111343.	2.7	5
27	Investigating Tetrel-Based Neutral Frustrated Lewis Pairs for Hydrogen Activation. <i>Inorganic Chemistry</i> , 2021, 60, 15180-15189.	1.9	9
28	Theoretical Insights into $\text{Na}_{5}\text{M}(\text{PO}_4)_2\text{F}_2$ (M = Cr, V): A Fluorophosphate-Based High-Performance Cathode System for Sodium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19593-19599.	1.5	3
29	Delineating Conformation Control in the Photophysical Behaviour of a Molecular Donor-Acceptor-Donor Triad. <i>ChemPhysChem</i> , 2021, 22, 2297-2304.	1.0	6
30	Multistimuli and fingertip-triggered luminescence switching: a five-colored ink-free rewritable secured platform with strongest red emission. <i>Journal of Materials Chemistry C</i> , 2021, 9, 9555-9570.	2.7	14
31	Bimetallic Zero-Valent Alloy with Measured High-Valent Surface States to Reinforce the Bifunctional Activity in Rechargeable Zinc-Air Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 14868-14880.	3.2	9
32	Assessing Tetrel-Based Neutral Frustrated Lewis Pairs for Catalytic Hydrogenation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22522-22530.	1.5	4
33	Explaining the Advantageous Impact of Tertiary versus Secondary Nitrogen Centre on the Activity of PNPincer Co(I) Complexes for Catalytic Hydrogenation of CO_2 . <i>Chemistry - A European Journal</i> , 2021, 27, 16407-16414.	1.7	3
34	Influence of N-heterocyclic carbenes (NHCs) on the hydrolysis of a diphosphene. <i>Dalton Transactions</i> , 2020, 49, 993-997.	1.6	7
35	High Capacity and High-Rate $\text{Na}_{3.75}\text{V}_{1.25}\text{Mn}_{0.75}(\text{PO}_4)_3$ Cathode for Na-Ion Batteries via Modulating Electronic and Crystal Structures. <i>Advanced Energy Materials</i> , 2020, 10, 1902918.	10.2	68
36	Facile One-Pot Assembly of Push-Pull Imines by a Selective C-F Substitution Process in Aryl Fluorides. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 7445-7449.	1.2	3

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37	Elusive Co ₂ O ₃ : A Combined Experimental and Theoretical Study. ACS Omega, 2020, 5, 29009-29016.	1.6	10
38	Metal fluorophosphate polyanionic insertion hosts as efficient bifunctional electrocatalysts for oxygen evolution and reduction reactions. Journal of Materials Chemistry A, 2020, 8, 18651-18658.	5.2	7
39	New Series of Pentanary Oxides, AM ₂ C ₆ Te ₃ O ₁₈ (A = Pb, Sr; M = Mn, Cd; C = Ni, Co): Synthesis, Structure, and Magnetic and Optical Properties. Journal of Physical Chemistry C, 2020, 124, 25071-25077.	1.5	1
40	An Annelated Mesoionic Carbene (MIC) Based Ru(II) Catalyst for Chemo- and Stereoselective Semihydrogenation of Internal and Terminal Alkynes. Organometallics, 2020, 39, 3212-3223.	1.1	16
41	Trisubstituted geminal diazaalkene derived transient 1,2-carbocations. Chemical Communications, 2020, 56, 8233-8236.	2.2	5
42	MOF Derived Co ₃ O ₄ @Co/NCNT Nanocomposite for Electrochemical Hydrogen Evolution, Flexible Zinc-Air Batteries, and Overall Water Splitting. Inorganic Chemistry, 2020, 59, 3160-3170.	1.9	67
43	Broadband Colossal Dielectric Constant in the Superionic Halide RbAg ₄ I ₅ : Role of Intercluster Ag ⁺ Diffusion. Journal of Physical Chemistry C, 2020, 124, 9802-9809.	1.5	4
44	Vibrational spectra of MO (M = Sn/Pb) in their bulk and single-layer forms: role of avoided crossing in their thermodynamic properties. Bulletin of Materials Science, 2020, 43, 1.	0.8	4
45	Semiconductivity and superhydrophobicity in an oligo-(p-phenyleneethynylene) (OPE)-based luminescent MOF. Bulletin of Materials Science, 2020, 43, 1.	0.8	1
46	Tuning of hyperpolarizability, and one- and two-photon absorption of donor-acceptor and donor-acceptor-acceptor-type intramolecular charge transfer-based sensors. Physical Chemistry Chemical Physics, 2019, 21, 17343-17355.	1.3	23
47	Red-Emitting Delayed Fluorescence and Room Temperature Phosphorescence from Core-Substituted Naphthalene Diimides. Chemistry - A European Journal, 2019, 25, 16007-16011.	1.7	34
48	Single pot synthesis of indirect band gap 2D CsPb ₂ Br ₅ nanosheets from direct band gap 3D CsPbBr ₃ nanocrystals and the origin of their luminescence properties. Nanoscale, 2019, 11, 4001-4007.	2.8	65
49	Phonon Localization and Entropy-Driven Point Defects Lead to Ultralow Thermal Conductivity and Enhanced Thermoelectric Performance in (SnTe) _{1-x} (SnSe) _x (SnS) _x . ACS Energy Letters, 2019, 4, 1658-1662.	8.8	70
50	Long-range ferromagnetism in nickel-based hybrid structure with semiconductor behavior. Chemical Communications, 2019, 55, 5211-5214.	2.2	4
51	N-Heterocyclic Germylene and Stannylene Catalyzed Cyanosilylation and Hydroboration of Aldehydes. Organometallics, 2019, 38, 1429-1435.	1.1	58
52	Effect of site energy fluctuation on charge transport in disordered organic molecules. Journal of Chemical Physics, 2019, 151, 224301.	1.2	9
53	Regulating Charge-Transfer in Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. Chemistry - A European Journal, 2019, 25, 3867-3874.	1.7	51
54	Laser Shock Tuning Dynamic Interlayer Coupling in Graphene-Boron Nitride Moiré Superlattices. Nano Letters, 2019, 19, 283-291.	4.5	31

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55	Redox-active and semi-conducting donor-acceptor conjugated microporous polymers as metal-free ORR catalysts. <i>Journal of Materials Chemistry A</i> , 2018, 6, 5587-5591.	5.2	69
56	Shining Light on New-Generation Two-Dimensional Materials from a Computational Viewpoint. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1605-1612.	2.1	22
57	Phosphorene quantum dots. <i>Chemical Physics Letters</i> , 2018, 699, 223-228.	1.2	29
58	Cobalt-Based Coordination Polymer for Oxygen Reduction Reaction. <i>ACS Omega</i> , 2018, 3, 3830-3834.	1.6	28
59	Mechanistic insights into catalytic CO ₂ hydrogenation using Mn(<i>scpi</i>)-complexes with pendant oxygen ligands. <i>Catalysis Science and Technology</i> , 2018, 8, 3034-3043.	2.1	13
60	Alpha Lead Oxide (α-PbO): A New 2D Material with Visible Light Sensitivity. <i>Small</i> , 2018, 14, e1703346.	5.2	58
61	Mechanistic Insights into Hydrogen Activation by Frustrated N/Sn Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 2575-2579.	1.7	21
62	Effects of point defects on the magnetoelectronic structures of MXenes from first principles. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4012-4019.	1.3	70
63	Covalently Functionalized Nanoparticles of Semiconducting Metal Chalcogenides and Their Attributes. <i>ChemNanoMat</i> , 2018, 4, 41-45.	1.5	4
64	Neutral and anionic phosphate-diester as molecular templates for the encapsulation of a water dimer. <i>Chemical Communications</i> , 2018, 54, 11913-11916.	2.2	12
65	Aqueous Phase Phosphorescence: Ambient Triplet Harvesting of Purely Organic Phosphors via Supramolecular Scaffolding. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 17115-17119.	7.2	101
66	Tailoring Ca ₂ Mn ₂ O ₅ Based Perovskites for Improved Oxygen Evolution Reaction. <i>ACS Applied Energy Materials</i> , 2018, 1, 6312-6319.	2.5	5
67	Theoretical modeling of charge transport in triphenylamine-benzimidazole based organic solids for their application as host-materials in phosphorescent OLEDs. <i>RSC Advances</i> , 2018, 8, 30021-30039.	1.7	9
68	Unravelling the mechanism of tin-based frustrated Lewis pair catalysed hydrogenation of carbonyl compounds. <i>Catalysis Science and Technology</i> , 2018, 8, 5178-5189.	2.1	10
69	Enhancing Selectivity and Kinetics in Oxidative Photocyclization by Supramolecular Control. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13662-13665.	7.2	20
70	Arsenene nanosheets and nanodots. <i>New Journal of Chemistry</i> , 2018, 42, 14091-14095.	1.4	62
71	Solvent-Modulated Emission Properties in a Superhydrophobic Oligo(p-phenyleneethynylene)-Based 3D Porous Supramolecular Framework. <i>Inorganic Chemistry</i> , 2018, 57, 8693-8696.	1.9	10
72	Theoretical insights into the excited-state properties of room-temperature phosphorescence-emitting N-substituted naphthalimides. <i>Journal of Molecular Modeling</i> , 2018, 24, 246.	0.8	4

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73	One-Step Simultaneous Exfoliation and Covalent Functionalization of MoS ₂ by Amino Acid Induced Solution Processes. <i>ChemNanoMat</i> , 2017, 3, 172-177.	1.5	33
74	Unique Approach to Copper(I) Silylene Chalcogenone Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 1706-1712.	1.9	39
75	Nanocomposites of C ₃ N ₄ with Layers of MoS ₂ and Nitrogenated RGO, Obtained by Covalent Cross-Linking: Synthesis, Characterization, and HER Activity. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 10664-10672.	4.0	118
76	Trapping of gaseous pollutants on defective N-doped graphene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 636-643.	1.3	10
77	Nanoscale Stabilization of Nonequilibrium Rock Salt BiAgSeS: Colloidal Synthesis and Temperature Driven Unusual Phase Transition. <i>Chemistry of Materials</i> , 2017, 29, 3769-3777.	3.2	16
78	Photocatalytic Activity of g-C ₃ N ₄ Quantum Dots in Visible Light: Effect of Physicochemical Modifications. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1982-1989.	1.5	68
79	Synthetically tuned structural variations in CePdxGe ₂ ^x (x = 0.21, 0.32, 0.69) towards diverse physical properties. <i>Inorganic Chemistry Frontiers</i> , 2017, 4, 241-255.	3.0	3
80	Colossal Increase in Electric Current and High Rectification Ratio in a Photoconducting, Self-Cleaning, and Luminescent Schottky Barrier NMOF Diode. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23803-23810.	1.5	23
81	Doping Phosphorene with Holes and Electrons through Molecular Charge Transfer. <i>ChemPhysChem</i> , 2017, 18, 2985-2989.	1.0	37
82	Superlinear amplification of the first hyperpolarizability of linear aggregates of DANS molecules. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24979-24984.	1.3	16
83	Trapping and sensing of hazardous insecticides by chemically modified single walled carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24059-24066.	1.3	7
84	Regulation of transport properties by polytypism: a computational study on bilayer MoS ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21282-21286.	1.3	3
85	On the Mechanism of Frustrated Lewis Pair Catalysed Hydrogenation of Carbonyl Compounds. <i>Chemistry - A European Journal</i> , 2017, 23, 1078-1085.	1.7	35
86	Breakdown of electron-pairs in the presence of an electric field of a superconducting ring. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 195601.	0.7	0
87	Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe ₂ . <i>Applied Physics Letters</i> , 2016, 109, .	1.5	25
88	Charge-transport anisotropy in black phosphorus: critical dependence on the number of layers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16345-16352.	1.3	17
89	Imidazolyl-Naphthalenediimide-Based Threading Intercalators of DNA. <i>ChemBioChem</i> , 2016, 17, 2162-2171.	1.3	22
90	Activity of Water Oxidation on Pure and (Fe, Ni, and Cu)-Substituted Co ₃ O ₄ . <i>ACS Energy Letters</i> , 2016, 1, 858-862.	8.8	59

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91	Role of donor-acceptor macrocycles in sequence specific peptide recognition and their optoelectronic properties: a detailed computational insight. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20682-20690.	1.3	4
92	Aggregates of quadrupolar dyes for two-photon absorption: the role of intermolecular interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28198-28208.	1.3	51
93	Electrochemical Dealloying of PdCu ₃ Nanoparticles to Achieve Pt-like Activity for the Hydrogen Evolution Reaction. <i>ChemSusChem</i> , 2016, 9, 2922-2927.	3.6	79
94	Optical Unzipping of Carbon Nanotubes in Liquid Media. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16985-16993.	1.5	21
95	Anodic performance of black phosphorus in magnesium-ion batteries: the significance of Mg-P bond-synergy. <i>Chemical Communications</i> , 2016, 52, 8381-8384.	2.2	40
96	Size-selective electrocatalytic activity of (Pt) _n /MoS ₂ for oxygen reduction reaction. <i>Catalysis Science and Technology</i> , 2016, 6, 6389-6395.	2.1	16
97	2D coordination polymer composed of 1D {NiII(1/4-O)(1/4-H2O)NiII} ferromagnetic chains: Modulation of magnetic properties based on dehydration and rehydration. <i>Polyhedron</i> , 2016, 115, 276-281.	1.0	4
98	Origin of the Order-Disorder Transition and the Associated Anomalous Change of Thermopower in AgBiS ₂ Nanocrystals: A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2016, 55, 6323-6331.	1.9	45
99	Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al ³⁺ Sensing. <i>Crystal Growth and Design</i> , 2016, 16, 82-91.	1.4	44
100	Spin-State Switching of Manganese Porphyrin by Conformational Modification. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3625-3634.	1.5	15
101	Phase Transition of MoS ₂ Bilayer Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3776-3780.	1.5	33
102	First-principles design of a borocarbonitride-based anode for superior performance in sodium-ion batteries and capacitors. <i>Journal of Materials Chemistry A</i> , 2016, 4, 5517-5527.	5.2	24
103	Surface-Mediated Extraction and Photoresponse Modulation of Bisphenol A Derivatives: A Computational Study. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 23893-23901.	4.0	4
104	Clean WS ₂ and MoS ₂ Nanoribbons Generated by Laser-Induced Unzipping of the Nanotubes. <i>Small</i> , 2015, 11, 3916-3920.	5.2	24
105	Highly Luminescent Microporous Organic Polymer with Lewis Acidic Boron Sites on the Pore Surface: Ratiometric Sensing and Capture of F ⁻ Ions. <i>Chemistry - A European Journal</i> , 2015, 21, 10799-10804.	1.7	55
106	Spin-crossover molecule based thermoelectric junction. <i>Applied Physics Letters</i> , 2015, 106, .	1.5	21
107	Sequence-specific recognition of DNA minor groove by an NIR-fluorescence switch-on probe and its potential applications. <i>Nucleic Acids Research</i> , 2015, 43, 8651-8663.	6.5	66
108	Photophysical properties of charge transfer pairs encapsulated inside macrocycle cage: A density functional theory study. <i>Chemical Physics Letters</i> , 2015, 624, 64-68.	1.2	4

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109	Linear and Nonlinear Optical Properties of Graphene Quantum Dots: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12079-12087.	1.5	78
110	Theoretical understanding of two-photon-induced fluorescence of isomorphous nucleoside analogs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10053-10058.	1.3	23
111	Watsonâ€™Crick base pairing, electronic and photophysical properties of triazole modified adenine analogues: a computational study. <i>New Journal of Chemistry</i> , 2015, 39, 9249-9256.	1.4	10
112	$\text{Eu}_{3}\text{Ir}_{2}\text{In}_{15}$: A Mixed-Valent and Vacancy-Filled Variant of the $\text{Sc}_{5}\text{Co}_{4}\text{Si}_{10}$ Structure Type with Anomalous Magnetic Properties. <i>Inorganic Chemistry</i> , 2015, 54, 10855-10864.	1.9	6
113	Criticality of surface topology for charge-carrier transport characteristics in two-dimensional borocarbonitrides: design principles for an efficient electronic material. <i>Nanoscale</i> , 2014, 6, 13430-13434.	2.8	15
114	Electronic properties of zigzag, armchair and their hybrid quantum dots of graphene and boron-nitride with and without substitution: A DFT study. <i>Chemical Physics Letters</i> , 2014, 603, 28-32.	1.2	25
115	BN-decorated graphene nanoflakes with tunable opto-electronic and charge transport properties. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2918-2928.	2.7	35
116	Line defects at the heterojunction of hybrid boron nitrideâ€™graphene nanoribbons. <i>Journal of Materials Chemistry C</i> , 2014, 2, 392-398.	2.7	23
117	A hexanuclear Cu_{6} cluster supported by cuprophilic interaction: effects of aromatics on luminescence properties. <i>RSC Advances</i> , 2014, 4, 35167-35170.	1.7	12
118	A probe for ratiometric near-infrared fluorescence and colorimetric hydrogen sulfide detection and imaging in live cells. <i>RSC Advances</i> , 2014, 4, 11147-11151.	1.7	64
119	Improved catalytic activity of rhodium monolayer modified nickel (110) surface for the methane dehydrogenation reaction: a first-principles study. <i>Nanoscale</i> , 2014, 6, 6738-6744.	2.8	13
120	Computational studies on magnetism and the optical properties of transition metal embedded graphitic carbon nitride sheets. <i>Journal of Materials Chemistry C</i> , 2014, 2, 7943-7951.	2.7	128
121	Possible application of 2D-boron sheets as anode material in lithium ion battery: A DFT and AIMD study. <i>Journal of Materials Chemistry A</i> , 2014, 2, 3856.	5.2	77
122	Transition Metal Embedded Two-Dimensional C_{3}N_{4} â€™Graphene Nanocomposite: A Multifunctional Material. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15487-15494.	1.5	93
123	Insertion of Line Defect in Nanoribbons of Graphene, Boron Nitride, and Hybrid of Them: An AIMD Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14670-14676.	1.5	9
124	Functional Corannulene: Diverse Structures, Enhanced Charge Transport, and Tunable Optoelectronic Properties. <i>ChemPhysChem</i> , 2014, 15, 885-893.	1.0	27
125	Effects of edge passivations on the electronic and magnetic properties of zigzag boron-nitride nanoribbons with even and odd-line stoneâ€™wales (5â€™7 pair) defects. <i>Indian Journal of Physics</i> , 2014, 88, 931-938.	0.9	3
126	Nitrogen-Doped Graphene Quantum Dots as Possible Substrates to Stabilize Planar Conformer of Au_{20} over Its Tetrahedral Conformer: A Systematic DFT Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17890-17894.	1.5	11

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127	Formation Mechanism and Possible Stereocontrol of Bisphenol A Derivatives: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9258-9262.	1.2	3
128	Structural and Magnetic Properties of a Variety of Transition Metal Incorporated DNA Double Helices. <i>Chemistry - A European Journal</i> , 2014, 20, 1760-1764.	1.7	12
129	Molecular Architectonics of Stereochemically Constrained Complementary Functional Modules. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5838-5847.	1.2	25
130	Adsorption of HF Pollutant on Single Vacant 2D Nanosheets: Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21700-21705.	1.5	18
131	Stability and electronic structure of carbon capsules with superior gas storage properties: A theoretical study. <i>Chemical Physics</i> , 2013, 426, 23-30.	0.9	8
132	Structural Stability, Electronic, Magnetic, and Optical Properties of Rectangular Graphene and Boron Nitride Quantum Dots: Effects of Size, Substitution, and Electric Field. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23295-23304.	1.5	50
133	Structural, electronic and photophysical properties of analogous RNA nucleosides: a theoretical study. <i>New Journal of Chemistry</i> , 2013, 37, 3640.	1.4	19
134	Tuning the electronic and optical properties of graphene and boron-nitride quantum dots by molecular charge-transfer interactions: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13881.	1.3	36
135	Theoretical understanding of single-stranded DNA assisted dispersion of graphene. <i>Journal of Materials Chemistry B</i> , 2013, 1, 91-100.	2.9	46
136	Computational Studies on Non-covalent Interactions of Carbon and Boron Fullerenes with Graphene. <i>ChemPhysChem</i> , 2013, 14, 1844-1852.	1.0	25
137	Effect of Imide Functionalization on the Electronic, Optical, and Charge Transport Properties of Coronene: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 825-836.	1.5	52
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