Swapan K Pati

List of Publications by Year
in descending order

264 papers	10,547 citations	34105 52 h-index	45317 90 g-index
269 all docs	269 docs citations	269 times ranked	13825 citing authors

#	Article	IF	Citations
1	Novel design of single transition metal atoms anchored on C6N6 nanosheet for electrochemical and photochemical N2 reduction to Ammonia. Catalysis Today, 2023, 424, 113804.	4.4	6
2	Loss of classicality in alternating spin- 12 /spin-1 chain, in the presence of next-neighbor couplings and Dzyaloshinskiiâ€"Moriya interactions. Journal of Physics Condensed Matter, 2022, 34, 175802.	1.8	0
3	Chiral Arylene Diimide Phosphors: Circularly Polarized Ambient Phosphorescence from Bischromophoric Pyromellitic Diimides. Angewandte Chemie - International Edition, 2022, 61, .	13.8	33
4	Polaronic Signatures in Doped and Undoped Cesium Lead Halide Perovskite Nanocrystals through a Photoinduced Raman Mode. ACS Applied Materials & Interfaces, 2022, 14, 5567-5577.	8.0	1
5	Activation of O₂ across a C(sp³)â€"C(sp³) bond. Chemical Communications, 2022, 58, 3122-3125.	4.1	0
6	Potassium Cobalt Pyrophosphate as a Nonprecious Bifunctional Electrocatalyst for Zincâ€"Air Batteries. ACS Applied Materials & Interfaces, 2022, 14, 8992-9001.	8.0	9
7	Impacts of CsPbBr₃/PbSe Heterostructures on Carrier Cooling Dynamics at Low Carrier Density. Advanced Optical Materials, 2022, 10, .	7.3	16
8	Influence of Noncovalent Interactions on the Magnetic Behavior of Three Isostructural Layered Manganese(II) Dicarboxylate-Based Coordination Polymers. Crystal Growth and Design, 2022, 22, 2534-2546.	3.0	6
9	Computational Insight into TMâ€"N_x Embedded Graphene Bifunctional Electrocatalysts for Oxygen Evolution and Reduction Reactions. ACS Physical Chemistry Au, 2022, 2, 305-315.	4.0	10
10	Recent Advances in Group 14 and 15 Lewis Acids for Frustrated Lewis Pair Chemistry. Chemistry - an Asian Journal, 2022, 17, .	3.3	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. Physical Chemistry Chemical Physics, 2022, 24, 10765-10774.	2.8	12
12	3dâ€Transition metal doped two-dimensional SnTe: Modulation of thermoelectric properties. Materials Today Communications, 2022, 31, 103656.	1.9	2
13	Anionâ"Ï€-Induced Room Temperature Phosphorescence from Emissive Charge-Transfer States. Journal of the American Chemical Society, 2022, 144, 10854-10861.	13.7	46
14	Modulating the Carrier Relaxation Dynamics in Heterovalently (Bi³⁺) Doped CsPbBr₃ Nanocrystals. Journal of Physical Chemistry Letters, 2022, 13, 5431-5440.	4.6	18
15	Unraveling the formation mechanism of NaCoPO4 polymorphs. Journal of Solid State Chemistry, 2021, 293, 121766.	2.9	4
16	Effect of conjugation on the vibrational modes of a carbon nanotube dimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 246, 118985.	3.9	4
17	Bicyclic (alkyl)(amino)carbene stabilized zinc(0) complex with singlet biradicaloid ground state. Chemical Communications, 2021, 57, 5282-5285.	4.1	14
18	A small heterocyclic molecule as a multistate transistor: a quantum many-body approach. Journal of Materials Chemistry C, 2021, 9, 10927-10934.	5.5	2

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19	Computational Exploration of Intramolecular Sn/N Frustrated Lewis Pairs for Hydrogen Activation and Catalytic Hydrogenation. Organometallics, 2021, 40, 194-202.	2.3	8
20	Exploring a Superlattice of SnO-PbO: A New Material for Thermoelectric Applications. ACS Applied Energy Materials, 2021, 4, 2081-2090.	5.1	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. Inorganic Chemistry, 2021, 60, 6911-6921.	4.0	17
22	Ambient Room Temperature Phosphorescence and Thermally Activated Delayed Fluorescence from a Core-Substituted Pyromellitic Diimide Derivative. Journal of Physical Chemistry B, 2021, 125, 4520-4526.	2.6	21
23	Arylene Diimide Phosphors: Aggregation Modulated Twin Room Temperature Phosphorescence from Pyromellitic Diimides. Angewandte Chemie - International Edition, 2021, 60, 12323-12327.	13.8	93
24	Lightâ€Harvesting Supramolecular Phosphors: Highly Efficient Room Temperature Phosphorescence in Solution and Hydrogels. Angewandte Chemie - International Edition, 2021, 60, 19720-19724.	13.8	135
25	Intersystem Crossing in Boron-Based Donorâ€"Spiroâ€"Acceptor Organic Chromophore: A Detailed Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 6674-6680.	2.5	15
26	Achievement of strain-driven ultrahigh carrier mobility in Î²-TeO2. Materials Research Bulletin, 2021, 141, 111343.	5.2	5
27	Investigating Tetrel-Based Neutral Frustrated Lewis Pairs for Hydrogen Activation. Inorganic Chemistry, 2021, 60, 15180-15189.	4.0	9
28	Theoretical Insights into Na₅M(PO₄)₂F₂ (M = Cr, V): A Fluorophosphate-Based High-Performance Cathode System for Sodium-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 19593-19599.	3.1	3
29	Delineating Conformation Control in the Photophysical Behaviour of a Molecular Donorâ€Acceptorâ€Donor Triad. ChemPhysChem, 2021, 22, 2297-2304.	2.1	6
30	Multistimuli and fingertip-triggered luminescence switching: a five-colored ink-free rewritable secured platform with strongest red emission. Journal of Materials Chemistry C, 2021, 9, 9555-9570.	5.5	14
31	Bimetallic Zero-Valent Alloy with Measured High-Valent Surface States to Reinforce the Bifunctional Activity in Rechargeable Zinc-Air Batteries. ACS Sustainable Chemistry and Engineering, 2021, 9, 14868-14880.	6.7	9
32	Assessing Tetrel-Based Neutral Frustrated Lewis Pairs for Catalytic Hydrogenation. Journal of Physical Chemistry C, 2021, 125, 22522-22530.	3.1	4
33	Explaining the Advantageous Impact of Tertiary versus Secondary Nitrogen Centre on the Activity of PNPâ€Pincer Co(I)â€Complexes for Catalytic Hydrogenation of CO2. Chemistry - A European Journal, 2021, 27, 16407-16414.	3.3	3
34	Influence of N-heterocyclic carbenes (NHCs) on the hydrolysis of a diphosphene. Dalton Transactions, 2020, 49, 993-997.	3.3	7
35	High Capacity and Highâ€Rate NASICONâ€Na_{3.75}V_{1.25}Mn_{0.75}(PO₄)₃ Cathode for Naâ€Ion Batteries via Modulating Electronic and Crystal Structures. Advanced Energy Materials, 2020, 10, 1902918.	19.5	68
36	Facile Oneâ€Pot Assembly of Pushâ€"Pull Imines by a Selective Câ€"F Substitution Process in Aryl Fluorides. European Journal of Organic Chemistry, 2020, 2020, 7445-7449.	2.4	3

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37	Elusive Co₂O₃: A Combined Experimental and Theoretical Study. ACS Omega, 2020, 5, 29009-29016.	3.5	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.	10.3	7
39	New Series of Pentanary Oxides, AM2C6Te3O18 (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.	3.1	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.	2.3	16
41	Trisubstituted geminal diazaalkene derived transient 1,2-carbodications. Chemical Communications, 2020, 56, 8233-8236.	4.1	5
42	MOF Derived Co₃O₄@Co/NCNT Nanocomposite for Electrochemical Hydrogen Evolution, Flexible Zinc-Air Batteries, and Overall Water Splitting. Inorganic Chemistry, 2020, 59, 3160-3170.	4.0	67
43	Broadband Colossal Dielectric Constant in the Superionic Halide RbAg₄I₅: Role of Intercluster Ag⁺ Diffusion. Journal of Physical Chemistry C, 2020, 124, 9802-9809.	3.1	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.	1.7	4
45	Semiconductivity and superhydrophobicity in an oligo-(p-phenyleneethynylene) (OPE)-based luminescent MOF. Bulletin of Materials Science, 2020, 43, 1.	1.7	1
46	Tuning of hyperpolarizability, and one- and two-photon absorption of donorâ€“acceptor and donorâ€“acceptorâ€“acceptor-type intramolecular charge transfer-based sensors. Physical Chemistry Chemical Physics, 2019, 21, 17343-17355.	2.8	23
47	Redâ€Emitting Delayed Fluorescence and Room Temperature Phosphorescence from Coreâ€Substituted Naphthalene Diimides. Chemistry - A European Journal, 2019, 25, 16007-16011.	3.3	34
48	Single pot synthesis of indirect band gap 2D CsPb₂Br₅nanosheets from direct band gap 3D CsPbBr₃nanocrystals and the origin of their luminescence properties. Nanoscale, 2019, 11, 4001-4007.	5.6	65
49	Phonon Localization and Entropy-Driven Point Defects Lead to Ultralow Thermal Conductivity and Enhanced Thermoelectric Performance in (SnTe)_{1â€“2x}(SnSe)_x(SnS)_x. ACS Energy Letters, 2019, 4, 1658-1662.	17.4	70
50	Long-range ferromagnetism in nickel-based hybrid structure with semiconductor behavior. Chemical Communications, 2019, 55, 5211-5214.	4.1	4
51	N-Heterocyclic Germylene and Stannylene Catalyzed Cyanosilylation and Hydroboration of Aldehydes. Organometallics, 2019, 38, 1429-1435.	2.3	58
52	Effect of site energy fluctuation on charge transport in disordered organic molecules. Journal of Chemical Physics, 2019, 151, 224301.	3.0	9
53	Regulating Chargeâ€Transfer in Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. Chemistry - A European Journal, 2019, 25, 3867-3874.	3.3	51
54	Laser Shock Tuning Dynamic Interlayer Coupling in Grapheneâ€“Boron Nitride MoirÃ© Superlattices. Nano Letters, 2019, 19, 283-291.	9.1	31

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55	Redox-active and semi-conducting donorâ€“acceptor conjugated microporous polymers as metal-free ORR catalysts. Journal of Materials Chemistry A, 2018, 6, 5587-5591.	10.3	69
56	Shining Light on New-Generation Two-Dimensional Materials from a Computational Viewpoint. Journal of Physical Chemistry Letters, 2018, 9, 1605-1612.	4.6	22
57	Phosphorene quantum dots. Chemical Physics Letters, 2018, 699, 223-228.	2.6	29
58	Cobalt-Based Coordination Polymer for Oxygen Reduction Reaction. ACS Omega, 2018, 3, 3830-3834.	3.5	28
59	Mechanistic insights into catalytic CO₂ hydrogenation using Mn(<scp>i</scp>)-complexes with pendant oxygen ligands. Catalysis Science and Technology, 2018, 8, 3034-3043.	4.1	13
60	Alpha Lead Oxide (Î±â€PbO): A New 2D Material with Visible Light Sensitivity. Small, 2018, 14, e1703346.	10.0	58
61	Mechanistic Insights into Hydrogen Activation by Frustrated N/Sn Lewis Pairs. Chemistry - A European Journal, 2018, 24, 2575-2579.	3.3	21
62	Effects of point defects on the magnetoelectronic structures of MXenes from first principles. Physical Chemistry Chemical Physics, 2018, 20, 4012-4019.	2.8	70
63	Covalently Functionalized Nanoparticles of Semiconducting Metal Chalcogenides and Their Attributes. ChemNanoMat, 2018, 4, 41-45.	2.8	4
64	Neutral and anionic phosphate-diesters as molecular templates for the encapsulation of a water dimer. Chemical Communications, 2018, 54, 11913-11916.	4.1	12
65	Aqueous Phase Phosphorescence: Ambient Triplet Harvesting of Purely Organic Phosphors via Supramolecular Scaffolding. Angewandte Chemie - International Edition, 2018, 57, 17115-17119.	13.8	101
66	Tailoring Ca₂Mn₂O₅ Based Perovskites for Improved Oxygen Evolution Reaction. ACS Applied Energy Materials, 2018, 1, 6312-6319.	5.1	5
67	Theoretical modeling of charge transport in triphenylamineâ€“benzimidazole based organic solids for their application as host-materials in phosphorescent OLEDs. RSC Advances, 2018, 8, 30021-30039.	3.6	9
68	Unravelling the mechanism of tin-based frustrated Lewis pair catalysed hydrogenation of carbonyl compounds. Catalysis Science and Technology, 2018, 8, 5178-5189.	4.1	10
69	Enhancing Selectivity and Kinetics in Oxidative Photocyclization by Supramolecular Control. Angewandte Chemie - International Edition, 2018, 57, 13662-13665.	13.8	20
70	Arsenene nanosheets and nanodots. New Journal of Chemistry, 2018, 42, 14091-14095.	2.8	62
71	Solvent-Modulated Emission Properties in a Superhydrophobic Oligo(p-phenyleneethynylene)-Based 3D Porous Supramolecular Framework. Inorganic Chemistry, 2018, 57, 8693-8696.	4.0	10
72	Theoretical insights into the excited-state properties of room-temperature phosphorescence-emitting N-substituted naphthalimides. Journal of Molecular Modeling, 2018, 24, 246.	1.8	4

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73	Oneâ€Step Simultaneous Exfoliation and Covalent Functionalization of MoS₂ by Amino Acid Induced Solution Processes. ChemNanoMat, 2017, 3, 172-177.	2.8	33
74	Unique Approach to Copper(I) Silylene Chalcogenone Complexes. Inorganic Chemistry, 2017, 56, 1706-1712.	4.0	39
75	Nanocomposites of C₃N₄with Layers of MoS₂and Nitrogenated RGO, Obtained by Covalent Cross-Linking: Synthesis, Characterization, and HER Activity. ACS Applied Materials & Interfaces, 2017, 9, 10664-10672.	8.0	118
76	Trapping of gaseous pollutants on defective N-doped graphene. Physical Chemistry Chemical Physics, 2017, 19, 636-643.	2.8	10
77	Nanoscale Stabilization of Nonequilibrium Rock Salt BiAgSeS: Colloidal Synthesis and Temperature Driven Unusual Phase Transition. Chemistry of Materials, 2017, 29, 3769-3777.	6.7	16
78	Photocatalytic Activity of g-C₃N₄ Quantum Dots in Visible Light: Effect of Physicochemical Modifications. Journal of Physical Chemistry C, 2017, 121, 1982-1989.	3.1	68
79	Synthetically tuned structural variations in CePdxGe2âˆ’x(x = 0.21, 0.32, 0.69) towards diverse physical properties. Inorganic Chemistry Frontiers, 2017, 4, 241-255.	6.0	3
80	Colossal Increase in Electric Current and High Rectification Ratio in a Photoconducting, Self-Cleaning, and Luminescent Schottky Barrier NMOF Diode. Journal of Physical Chemistry C, 2017, 121, 23803-23810.	3.1	23
81	Doping Phosphorene with Holes and Electrons through Molecular Charge Transfer. ChemPhysChem, 2017, 18, 2985-2989.	2.1	37
82	Superlinear amplification of the first hyperpolarizability of linear aggregates of DANS molecules. Physical Chemistry Chemical Physics, 2017, 19, 24979-24984.	2.8	16
83	Trapping and sensing of hazardous insecticides by chemically modified single walled carbon nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 24059-24066.	2.8	7
84	Regulation of transport properties by polytypism: a computational study on bilayer MoS2. Physical Chemistry Chemical Physics, 2017, 19, 21282-21286.	2.8	3
85	On the Mechanism of Frustrated Lewis Pair Catalysed Hydrogenation of Carbonyl Compounds. Chemistry - A European Journal, 2017, 23, 1078-1085.	3.3	35
86	Breakdown of electron-pairs in the presence of an electric field of a superconducting ring. Journal of Physics Condensed Matter, 2016, 28, 195601.	1.8	0
87	Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe2. Applied Physics Letters, 2016, 109, .	3.3	25
88	Charge-transport anisotropy in black phosphorus: critical dependence on the number of layers. Physical Chemistry Chemical Physics, 2016, 18, 16345-16352.	2.8	17
89	Imidazolylâ€Naphthalenediimideâ€Based Threading Intercalators of DNA. ChemBioChem, 2016, 17, 2162-2171.	2.6	22
90	Activity of Water Oxidation on Pure and (Fe, Ni, and Cu)-Substituted Co₃O₄. ACS Energy Letters, 2016, 1, 858-862.	17.4	59

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91	Role of donorâ€“acceptor macrocycles in sequence specific peptide recognition and their optoelectronic properties: a detailed computational insight. Physical Chemistry Chemical Physics, 2016, 18, 20682-20690.	2.8	4
92	Aggregates of quadrupolar dyes for two-photon absorption: the role of intermolecular interactions. Physical Chemistry Chemical Physics, 2016, 18, 28198-28208.	2.8	51
93	Electrochemical Dealloying of PdCu₃ Nanoparticles to Achieve Ptâ€like Activity for the Hydrogen Evolution Reaction. ChemSusChem, 2016, 9, 2922-2927.	6.8	79
94	Optical Unzipping of Carbon Nanotubes in Liquid Media. Journal of Physical Chemistry C, 2016, 120, 16985-16993.	3.1	21
95	Anodic performance of black phosphorus in magnesium-ion batteries: the significance of Mgâ€“P bond-synergy. Chemical Communications, 2016, 52, 8381-8384.	4.1	40
96	Size-selective electrocatalytic activity of (Pt)_n/MoS₂ for oxygen reduction reaction. Catalysis Science and Technology, 2016, 6, 6389-6395.	4.1	16
97	2D coordination polymer composed of 1D {NiII(Î¼-O)(Î¼-H2O)NiII} ferromagnetic chains: Modulation of magnetic properties based on dehydration and rehydration. Polyhedron, 2016, 115, 276-281.	2.2	4
98	Origin of the Orderâ€“Disorder Transition and the Associated Anomalous Change of Thermopower in AgBiS₂ Nanocrystals: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2016, 55, 6323-6331.	4.0	45
99	Luminescent Metalâ€“Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al³⁺ Sensing. Crystal Growth and Design, 2016, 16, 82-91.	3.0	44
100	Spin-State Switching of Manganese Porphyrin by Conformational Modification. Journal of Physical Chemistry C, 2016, 120, 3625-3634.	3.1	15
101	Phase Transition of MoS₂ Bilayer Structures. Journal of Physical Chemistry C, 2016, 120, 3776-3780.	3.1	33
102	First-principles design of a borocarbonitride-based anode for superior performance in sodium-ion batteries and capacitors. Journal of Materials Chemistry A, 2016, 4, 5517-5527.	10.3	24
103	Surface-Mediated Extraction and Photoresponse Modulation of Bisphenol A Derivatives: A Computational Study. ACS Applied Materials & Interfaces, 2015, 7, 23893-23901.	8.0	4
104	Clean WS₂ and MoS₂ Nanoribbons Generated by Laserâ€Induced Unzipping of the Nanotubes. Small, 2015, 11, 3916-3920.	10.0	24
105	Highly Luminescent Microporous Organic Polymer with Lewis Acidic Boron Sites on the Pore Surface: Ratiometric Sensing and Capture of F^{â’} Ions. Chemistry - A European Journal, 2015, 21, 10799-10804.	3.3	55
106	Spin-crossover molecule based thermoelectric junction. Applied Physics Letters, 2015, 106, .	3.3	21
107	Sequence-specific recognition of DNA minor groove by an NIR-fluorescence switch-on probe and its potential applications. Nucleic Acids Research, 2015, 43, 8651-8663.	14.5	66
108	Photophysical properties of charge transfer pairs encapsulated inside macrocycle cage: A density functional theory study. Chemical Physics Letters, 2015, 624, 64-68.	2.6	4

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109	Linear and Nonlinear Optical Properties of Graphene Quantum Dots: A Computational Study. Journal of Physical Chemistry C, 2015, 119, 12079-12087.	3.1	78
110	Theoretical understanding of two-photon-induced fluorescence of isomorphic nucleoside analogs. Physical Chemistry Chemical Physics, 2015, 17, 10053-10058.	2.8	23
111	Watsonâ€"Crick base pairing, electronic and photophysical properties of triazole modified adenine analogues: a computational study. New Journal of Chemistry, 2015, 39, 9249-9256.	2.8	10
112	Eu₃Ir₂In₁₅: A Mixed-Valent and Vacancy-Filled Variant of the Sc₅Co₄Si₁₀ Structure Type with Anomalous Magnetic Properties. Inorganic Chemistry, 2015, 54, 10855-10864.	4.0	6
113	Criticality of surface topology for charge-carrier transport characteristics in two-dimensional borocarbonitrides: design principles for an efficient electronic material. Nanoscale, 2014, 6, 13430-13434.	5.6	15
114	Electronic properties of zigzag, armchair and their hybrid quantum dots of graphene and boron-nitride with and without substitution: A DFT study. Chemical Physics Letters, 2014, 603, 28-32.	2.6	25
115	BN-decorated graphene nanoflakes with tunable opto-electronic and charge transport properties. Journal of Materials Chemistry C, 2014, 2, 2918-2928.	5.5	35
116	Line defects at the heterojunction of hybrid boron nitrideâ€"graphene nanoribbons. Journal of Materials Chemistry C, 2014, 2, 392-398.	5.5	23
117	A hexanuclear Cu(<scp>i</scp>) cluster supported by cuprophilic interaction: effects of aromatics on luminescence properties. RSC Advances, 2014, 4, 35167-35170.	3.6	12
118	A probe for ratiometric near-infrared fluorescence and colorimetric hydrogen sulfide detection and imaging in live cells. RSC Advances, 2014, 4, 11147-11151.	3.6	64
119	Improved catalytic activity of rhodium monolayer modified nickel (110) surface for the methane dehydrogenation reaction: a first-principles study. Nanoscale, 2014, 6, 6738-6744.	5.6	13
120	Computational studies on magnetism and the optical properties of transition metal embedded graphitic carbon nitride sheets. Journal of Materials Chemistry C, 2014, 2, 7943-7951.	5.5	128
121	Possible application of 2D-boron sheets as anode material in lithium ion battery: A DFT and AIMD study. Journal of Materials Chemistry A, 2014, 2, 3856.	10.3	77
122	Transition Metal Embedded Two-Dimensional C₃N₄â€"Graphene Nanocomposite: A Multifunctional Material. Journal of Physical Chemistry C, 2014, 118, 15487-15494.	3.1	93
123	Insertion of Line Defect in Nanoribbons of Graphene, Boron Nitride, and Hybrid of Them: An AIMD Study. Journal of Physical Chemistry C, 2014, 118, 14670-14676.	3.1	9
124	Functional Corannulene: Diverse Structures, Enhanced Charge Transport, and Tunable Optoelectronic Properties. ChemPhysChem, 2014, 15, 885-893.	2.1	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. Indian Journal of Physics, 2014, 88, 931-938.	1.8	3
126	Nitrogen-Doped Graphene Quantum Dots as Possible Substrates to Stabilize Planar Conformer of Au₂₀ over Its Tetrahedral Conformer: A Systematic DFT Study. Journal of Physical Chemistry C, 2014, 118, 17890-17894.	3.1	11

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127	Formation Mechanism and Possible Stereocontrol of Bisphenol A Derivatives: A Computational Study. Journal of Physical Chemistry B, 2014, 118, 9258-9262.	2.6	3
128	Structural and Magnetic Properties of a Variety of Transition Metal Incorporated DNA Double Helices. Chemistry - A European Journal, 2014, 20, 1760-1764.	3.3	12
129	Molecular Architectonics of Stereochemically Constrained Ï€â€Complementary Functional Modules. European Journal of Organic Chemistry, 2013, 2013, 5838-5847.	2.4	25
130	Adsorption of HF Pollutant on Single Vacant 2D Nanosheets: Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2013, 117, 21700-21705.	3.1	18
131	Stability and electronic structure of carbon capsules with superior gas storage properties: A theoretical study. Chemical Physics, 2013, 426, 23-30.	1.9	8
132	Structural Stability, Electronic, Magnetic, and Optical Properties of Rectangular Graphene and Boron Nitride Quantum Dots: Effects of Size, Substitution, and Electric Field. Journal of Physical Chemistry C, 2013, 117, 23295-23304.	3.1	50
133	Structural, electronic and photophysical properties of analogous RNA nucleosides: a theoretical study. New Journal of Chemistry, 2013, 37, 3640.	2.8	19
134	Tuning the electronic and optical properties of graphene and boron-nitride quantum dots by molecular charge-transfer interactions: a theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 13881.	2.8	36
135	Theoretical understanding of single-stranded DNA assisted dispersion of graphene. Journal of Materials Chemistry B, 2013, 1, 91-100.	5.8	46
136	Computational Studies on Nonâ€covalent Interactions of Carbon and Boron Fullerenes with Graphene. ChemPhysChem, 2013, 14, 1844-1852.	2.1	25
137	Effect of Imide Functionalization on the Electronic, Optical, and Charge Transport Properties of Coronene: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 825-836.	3.1	52
138	Effect of edge states on the electronic, magnetic and transport properties of BN-fused polyacene zigzag nanoribbons. Journal of Materials Chemistry C, 2013, 1, 3439.	5.5	12
139	Methane formation from the hydrogenation of carbon dioxide on Ni(110) surface â€“ a density functional theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 5701.	2.8	34
140	Density functional theoretical investigation on structure, optical response and hydrogen adsorption properties of B9/metalâ€“B9 clusters. Physical Chemistry Chemical Physics, 2013, 15, 8303.	2.8	10
141	Electronic and Magnetic Properties of Zigzag Boron-Nitride Nanoribbons with Even and Odd-Line Stone-Wales (5â€“7 Pair) Defects. Journal of Physical Chemistry C, 2013, 117, 3580-3594.	3.1	22
142	DESIGNING TUNABLE ELECTRONIC AND MAGNETIC PROPERTIES OF GRAPHENE: A THEORETICAL PERSPECTIVE. International Journal of Modern Physics B, 2012, 26, 1242003.	2.0	3
143	Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study. Journal of Physical Chemistry B, 2012, 116, 14754-14759.	2.6	20
144	Electronic, Magnetic, and Transport Properties of Fe_n-bis(n-acene) and Fe_n-bis(n-BNacene) [n = 1,2,â‹¯]: A Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 18487-18494.	3.1	9

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145	Computational studies on structural and optical properties of single-stranded DNA encapsulated silver/gold clusters. Journal of Materials Chemistry, 2012, 22, 6774.	6.7	20
146	First principles calculation on the structure and electronic properties of BNNTs functionalized with isoniazid drug molecule. Applied Nanoscience (Switzerland), 2012, 2, 389-400.	3.1	52
147	Cyclopentadienylâ€“benzene based sandwich molecular wires showing efficient spin filtering, negative differential resistance, and pressure induced electronic transitions. Journal of Materials Chemistry, 2012, 22, 14916.	6.7	30
148	Thieno Analogues of RNA Nucleosides: A Detailed Theoretical Study. Journal of Physical Chemistry B, 2012, 116, 7618-7626.	2.6	39
149	The interaction of halogen molecules with SWNTs and graphene. RSC Advances, 2012, 2, 1181-1188.	3.6	33
150	Beyond the FÃ¶rster formulation for resonance energy transfer: the role of dark states. Physical Chemistry Chemical Physics, 2011, 13, 12734.	2.8	18
151	Tunable Electronic and Magnetic Properties in B_xN_yC_z Nanohybrids: Effect of Domain Segregation. Journal of Physical Chemistry C, 2011, 115, 10842-10850.	3.1	97
152	Computational Studies on Structural and Excited-State Properties of Modified Chlorophyll f with Various Axial Ligands. Journal of Physical Chemistry A, 2011, 115, 12298-12306.	2.5	14
153	Density functional theoretical investigation of the aromatic nature of BN substituted benzene and four ring polyaromatic hydrocarbons. Physical Chemistry Chemical Physics, 2011, 13, 20627.	2.8	48
154	Interaction of Inorganic Nanoparticles with Graphene. ChemPhysChem, 2011, 12, 937-943.	2.1	72
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