

# Swapan K Pati

## List of Publications by Year in descending order

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264  
papers

10,547  
citations

34016

52  
h-index

45213

90  
g-index

269  
all docs

269  
docs citations

269  
times ranked

13825  
citing authors

#	ARTICLE	IF	CITATIONS
1	MoS <sub>2</sub> and WS <sub>2</sub> Analogues of Graphene. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 4059-4062.	7.2	1,417
2	Novel properties of graphene nanoribbons: a review. <i>Journal of Materials Chemistry</i> , 2010, 20, 8207.	6.7	369
3	Uptake of H <sub>2</sub> and CO <sub>2</sub> by Graphene. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15704-15707.	1.5	288
4	A study of graphene decorated with metal nanoparticles. <i>Chemical Physics Letters</i> , 2010, 497, 70-75.	1.2	286
5	Dipolar interactions and hydrogen bonding in supramolecular aggregates: understanding cooperative phenomena for 1st hyperpolarizability. <i>Chemical Society Reviews</i> , 2006, 35, 1305.	18.7	227
6	Density-matrix renormalization-group studies of the spin-1/2 Heisenberg system with dimerization and frustration. <i>Physical Review B</i> , 1995, 52, 6581-6587.	1.1	215
7	Half-Metallicity in Undoped and Boron Doped Graphene Nanoribbons in the Presence of Semilocal Exchange-Correlation Interactions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1333-1335.	1.2	188
8	Low-lying excited states and low-temperature properties of an alternating spin-1 spin-1/2 chain: A density-matrix renormalization-group study. <i>Physical Review B</i> , 1997, 55, 8894-8904.	1.1	180
9	Visible-Near-Infrared and Fluorescent Copper Sensors Based on Julolidine Conjugates: Selective Detection and Fluorescence Imaging in Living Cells. <i>Chemistry - A European Journal</i> , 2011, 17, 11152-11161.	1.7	173
10	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
11	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
12	Nanocomposites of C <sub>3</sub> N <sub>4</sub> with Layers of MoS <sub>2</sub> and Nitrogenated RGO, Obtained by Covalent Cross-Linking: Synthesis, Characterization, and HER Activity. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 10664-10672.	4.0	118
13	Dipole orientation effects on nonlinear optical properties of organic molecular aggregates. <i>Journal of Chemical Physics</i> , 2003, 118, 8420-8427.	1.2	117
14	Alternating Spin and Orbital Dimerization and Spin-Gap Formation in Coupled Spin-Orbital Systems. <i>Physical Review Letters</i> , 1998, 81, 5406-5409.	2.9	112
15	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
16	Conformationally Tuned Large Two-Photon Absorption Cross Sections in Simple Molecular Chromophores. <i>Journal of the American Chemical Society</i> , 2001, 123, 7287-7291.	6.6	100
17	Tunable Electronic and Magnetic Properties in B <sub>x</sub> N <sub>y</sub> C <sub>z</sub> Nanohybrids: Effect of Domain Segregation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10842-10850.	1.5	97
18	Transition Metal Embedded Two-Dimensional C <sub>3</sub> N <sub>4</sub> Graphene Nanocomposite: A Multifunctional Material. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15487-15494.	1.5	93

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19	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
20	Electrochemical Dealloying of PdCu <sub>3</sub> Nanoparticles to Achieve Pt-like Activity for the Hydrogen Evolution Reaction. <i>ChemSusChem</i> , 2016, 9, 2922-2927.	3.6	79
21	Electron and hole mobilities in polymorphs of benzene and naphthalene: Role of intermolecular interactions. <i>Journal of Chemical Physics</i> , 2007, 126, 144710.	1.2	78
22	Synthesis, structure and properties of homogeneous BC <sub>4</sub> N nanotubes. <i>Journal of Materials Chemistry</i> , 2008, 18, 83-90.	6.7	78
23	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
24	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
25	Symmetrized density-matrix renormalization-group method for excited states of Hubbard models. <i>Physical Review B</i> , 1996, 54, 7598-7601.	1.1	74
26	Interaction of Inorganic Nanoparticles with Graphene. <i>ChemPhysChem</i> , 2011, 12, 937-943.	1.0	72
27	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
28	Phonon Localization and Entropy-Driven Point Defects Lead to Ultralow Thermal Conductivity and Enhanced Thermoelectric Performance in (SnTe) <sub>1-x</sub> (SnSe) <sub>x</sub> (SnS) <sub>x</sub> . <i>ACS Energy Letters</i> , 2019, 4, 1658-1662.	8.8	70
29	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
30	Charge-Transfer Induced Large Nonlinear Optical Properties of Small Al Clusters: Al <sub>4</sub> M <sub>4</sub> (M = Li, Na). <i>Tj ETQq0.0 rgBT /Overlock 1</i>	1.1	68
31	Photocatalytic Activity of g-C <sub>3</sub> N <sub>4</sub> Quantum Dots in Visible Light: Effect of Physicochemical Modifications. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1982-1989.	1.5	68
32	High Capacity and High-Rate NASICON <sub>3.75</sub> V <sub>1.25</sub> Mn <sub>0.75</sub> (PO <sub>4</sub> ) <sub>3</sub> Cathode for Na-Ion Batteries via Modulating Electronic and Crystal Structures. <i>Advanced Energy Materials</i> , 2020, 10, 1902918.	10.2	68
33	Comparing the electron and hole mobilities in the $\hat{1}\pm$ and $\hat{1}^2$ phases of perylene: role of $\hat{I}$ -stacking. <i>Journal of Materials Chemistry</i> , 2007, 17, 1933-1938.	6.7	67
34	MOF Derived Co <sub>3</sub> O <sub>4</sub> @Co/NCNT Nanocomposite for Electrochemical Hydrogen Evolution, Flexible Zinc-Air Batteries, and Overall Water Splitting. <i>Inorganic Chemistry</i> , 2020, 59, 3160-3170.	1.9	67
35	Competing Magnetic Interactions in a Dinuclear Ni(II) Complex: Antiferromagnetic O $\hat{A}$ ~H $\hat{A}$ ~ $\hat{A}$ ~O Moiety and Ferromagnetic N <sub>3</sub> -Ligand. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12-15.	1.2	66
36	Molecular Electronics: Effect of External Electric Field. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14718-14730.	1.5	66

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37	Toward DNA Conductivity: A Theoretical Perspective. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1881-1894.	2.1	66
38	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
39	Single pot synthesis of indirect band gap 2D CsPb <sub>2</sub> Br <sub>5</sub> nanosheets from direct band gap 3D CsPbBr <sub>3</sub> nanocrystals and the origin of their luminescence properties. <i>Nanoscale</i> , 2019, 11, 4001-4007.	2.8	65
40	Ambipolar Charge Transport in $\hat{\pi}$ -Oligofurans: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20436-20442.	1.5	64
41	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
42	Arsenene nanosheets and nanodots. <i>New Journal of Chemistry</i> , 2018, 42, 14091-14095.	1.4	62
43	Conformational Tuning of Magnetic Interactions in Metal-DNA Complexes. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4977-4981.	7.2	61
44	Activity of Water Oxidation on Pure and (Fe, Ni, and Cu)-Substituted Co <sub>3</sub> O <sub>4</sub> . <i>ACS Energy Letters</i> , 2016, 1, 858-862.	8.8	59
45	Alpha Lead Oxide ( $\hat{\pi}$ -PbO): A New 2D Material with Visible Light Sensitivity. <i>Small</i> , 2018, 14, e1703346.	5.2	58
46	N-Heterocyclic Germylene and Stannylene Catalyzed Cyanosilylation and Hydroboration of Aldehydes. <i>Organometallics</i> , 2019, 38, 1429-1435.	1.1	58
47	Stable Transition Metal Complexes of an All-Metal Antiaromatic Molecule (Al <sub>4</sub> Li <sub>4</sub> ): A Role of Complexations. <i>Journal of the American Chemical Society</i> , 2005, 127, 3496-3500.	6.6	56
48	Low-lying electronic excitations and nonlinear optic properties of polymers via symmetrized density matrix renormalization group method. <i>Synthetic Metals</i> , 1997, 85, 1019-1022.	2.1	55
49	Magnetization properties of some quantum spin ladders. <i>Physical Review B</i> , 1999, 59, 396-410.	1.1	55
50	Highly Luminescent Microporous Organic Polymer with Lewis Acidic Boron Sites on the Pore Surface: Ratiometric Sensing and Capture of F <sup>-</sup> Ions. <i>Chemistry - A European Journal</i> , 2015, 21, 10799-10804.	1.7	55
51	Quantifying Aromaticity at the Molecular and Supramolecular Limits: Comparing Homonuclear, Heteronuclear, and H-Bonded Systems. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 30-36.	2.3	54
52	Organometallic vanadium-borazine systems: efficient one-dimensional half-metallic spin filters. <i>Journal of Materials Chemistry</i> , 2009, 19, 1761-1766.	6.7	53
53	First principles calculation on the structure and electronic properties of BNNTs functionalized with isoniazid drug molecule. <i>Applied Nanoscience (Switzerland)</i> , 2012, 2, 389-400.	1.6	52
54	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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55	Large carrier mobilities in octathio[8]circulene crystals: a theoretical study. <i>Journal of Materials Chemistry</i> , 2009, 19, 4356.	6.7	51
56	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
57	Regulating Charge Transfer in Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. <i>Chemistry - A European Journal</i> , 2019, 25, 3867-3874.	1.7	51
58	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
59	Nonlocal Electronic Distribution in Metallic Clusters: A Critical Examination of Aromatic Stabilization. <i>Accounts of Chemical Research</i> , 2007, 40, 213-221.	7.6	49
60	Density functional theoretical investigation of the aromatic nature of BN substituted benzene and four ring polyaromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20627.	1.3	48
61	Dynamical nonlinear optical coefficients from the symmetrized density-matrix renormalization-group method. <i>Physical Review B</i> , 1999, 59, 14827-14830.	1.1	47
62	Computational Design of High Hydrogen Adsorption Efficiency in Molecular Sulfur. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4487-4490.	1.5	47
63	Vanadium Benzimidazole-Modified sDNA: A One-Dimensional Half-Metallic Ferromagnet. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13877-13880.	1.2	46
64	Theoretical understanding of single-stranded DNA assisted dispersion of graphene. <i>Journal of Materials Chemistry B</i> , 2013, 1, 91-100.	2.9	46
65	Anion-Induced Room Temperature Phosphorescence from Emissive Charge-Transfer States. <i>Journal of the American Chemical Society</i> , 2022, 144, 10854-10861.	6.6	46
66	A density matrix renormalization group study of low-energy excitations and low-temperature properties of alternating spin systems. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 8707-8726.	0.7	45
67	Binding energy of singlet excitons in the one-dimensional extended Hubbard-Peierls model. <i>Physical Review B</i> , 1997, 55, 15368-15371.	1.1	45
68	Origin of the Order-Disorder Transition and the Associated Anomalous Change of Thermopower in AgBiS <sub>2</sub> Nanocrystals: A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2016, 55, 6323-6331.	1.9	45
69	Edge reconstructions induce magnetic and metallic behavior in zigzag graphene nanoribbons. <i>Carbon</i> , 2010, 48, 4409-4413.	5.4	44
70	Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al <sup>3+</sup> Sensing. <i>Crystal Growth and Design</i> , 2016, 16, 82-91.	1.4	44
71	Effects of Dipole Orientations on Nonlinear Optical Properties of Oxo-Bridged Dinitroaniline Systems. <i>Journal of Physical Chemistry A</i> , 2004, 108, 320-325.	1.1	43
72	Quantum-confinement effects on the ordering of the lowest-lying excited states in conjugated chains. <i>Physical Review B</i> , 1997, 56, 9298-9301.	1.1	42

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73	Ring currents in condensed ring systems. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 503-513.	1.0	42
74	Inorganic-Organic Hybrid Compounds: Synthesis, Structure, and Magnetic Properties of the First Organically Templated Iron Oxalate-Phosphite, $[C_4N_2H_{12}][Fe^{II}_4(HPO_3)_2(C_2O_4)_3]$ , Possessing Infinite $Fe-O-Fe$ Chains. <i>Chemistry of Materials</i> , 2005, 17, 2912-2917.	3.2	42
75	The First One-Dimensional Iron Phosphite-Phosphate, $[Fe^{III}(2,2\text{-bipyridine})(HPO_3)(H_2PO_4)]$ : Synthesis, Structure, and Magnetic Properties. <i>Chemistry of Materials</i> , 2005, 17, 638-643.	3.2	41
76	Role of Triple Bond in 1,2-Diphenylacetylene Crystal: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24674-24677.	1.2	41
77	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
78	Thieno Analogues of RNA Nucleosides: A Detailed Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7618-7626.	1.2	39
79	Unique Approach to Copper(I) Silylene Chalcogenone Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 1706-1712.	1.9	39
80	Doping Phosphorene with Holes and Electrons through Molecular Charge Transfer. <i>ChemPhysChem</i> , 2017, 18, 2985-2989.	1.0	37
81	Discordant Gd and Electronic Band Flattening Synergistically Induce High Thermoelectric Performance in n-type PbTe. <i>ACS Energy Letters</i> , 0, , 1625-1632.	8.8	37
82	Structures of Nucleobases Trapped within Au Triangles and Its Effects on Hydrogen Bonding in Base Pairs of DNA. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18661-18664.	1.2	36
83	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
84	Nonlinear Optical Properties in Calix[n]arenes: Orientation Effects of Monomers. <i>Chemistry - A European Journal</i> , 2005, 11, 4961-4969.	1.7	35
85	Sequence Dependent Electron Transport in Wet DNA: Ab Initio and Molecular Dynamics Studies. <i>Physical Review Letters</i> , 2008, 101, 176805.	2.9	35
86	On Nitrogen Insertion of a Diazo Compound into a Germanium(II) Hydrogen Bond and a Comparable Reaction with Diethyl Azodicarboxylate. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4246-4248.	7.2	35
87	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
88	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
89	Observation of tancoite-like chains in a one-dimensional metal-organic polymer. <i>Journal of Materials Chemistry</i> , 2003, 13, 2937-2941.	6.7	34
90	Doping single-walled carbon nanotubes through molecular charge-transfer: a theoretical study. <i>Nanoscale</i> , 2010, 2, 1190.	2.8	34

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91	Methane formation from the hydrogenation of carbon dioxide on Ni(110) surface – a density functional theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5701.	1.3	34
92	Red-Emitting Delayed Fluorescence and Room Temperature Phosphorescence from Core-Substituted Naphthalene Diimides. <i>Chemistry - A European Journal</i> , 2019, 25, 16007-16011.	1.7	34
93	The interaction of halogen molecules with SWNTs and graphene. <i>RSC Advances</i> , 2012, 2, 1181-1188.	1.7	33
94	Phase Transition of MoS <sub>2</sub> Bilayer Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3776-3780.	1.5	33
95	One-Step Simultaneous Exfoliation and Covalent Functionalization of MoS <sub>2</sub> by Amino Acid Induced Solution Processes. <i>ChemNanoMat</i> , 2017, 3, 172-177.	1.5	33
96	Chiral Arylene Diimide Phosphors: Circularly Polarized Ambient Phosphorescence from Bischromophoric Pyromellitic Diimides. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	33
97	Aromaticity in Stable Tiara Nickel Thiolates: Computational and Structural Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11647-11649.	1.1	32
98	Current-voltage characteristics in donor-acceptor systems: Implications of a spatially varying electric field. <i>Physical Review B</i> , 2005, 72, .	1.1	31
99	Semiconductor to metal transition in SWNTs caused by interaction with gold and platinum nanoparticles. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 215211.	0.7	31
100	Laser Shock Tuning Dynamic Interlayer Coupling in Graphene-Boron Nitride Moiré Superlattices. <i>Nano Letters</i> , 2019, 19, 283-291.	4.5	31
101	Magnetic Interactions in Layered Nickel Alkanethiolates. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1868-1870.	1.5	30
102	Cyclopentadienyl-benzene based sandwich molecular wires showing efficient spin filtering, negative differential resistance, and pressure induced electronic transitions. <i>Journal of Materials Chemistry</i> , 2012, 22, 14916.	6.7	30
103	Phosphorene quantum dots. <i>Chemical Physics Letters</i> , 2018, 699, 223-228.	1.2	29
104	Effect of electron-phonon coupling on the conductance of a one-dimensional molecular wire. <i>Journal of Chemical Physics</i> , 2004, 121, 11998-12004.	1.2	28
105	Cobalt-Based Coordination Polymer for Oxygen Reduction Reaction. <i>ACS Omega</i> , 2018, 3, 3830-3834.	1.6	28
106	Role of the spin magnitude of the magnetic ion in determining the frustration and low-temperature properties of kagome lattices. <i>Journal of Chemical Physics</i> , 2005, 123, 234703.	1.2	27
107	Functional Corannulene: Diverse Structures, Enhanced Charge Transport, and Tunable Optoelectronic Properties. <i>ChemPhysChem</i> , 2014, 15, 885-893.	1.0	27
108	Symmetrized density matrix renormalization group studies of the properties of low-lying states of the poly-para-phenylene system. <i>Journal of Chemical Physics</i> , 1997, 106, 10230-10237.	1.2	26



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109	Gapless singlet modes in the kagomé strips: A study through density-matrix-renormalization group and strong-coupling analysis. <i>Physical Review B</i> , 1999, 60, 7695-7698.	1.1	25
110	Rationalization of the $\pi$ (Anti)aromaticity in All Metal Molecular Clusters. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 824-826.	2.3	25
111	Structure and Transport Characteristics of Modified DNA with Magnetic Ions. <i>Physical Review Letters</i> , 2007, 98, 136601.	2.9	25
112	Molecular Architectonics of Stereochemically Constrained $\pi$ -Complementary Functional Modules. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5838-5847.	1.2	25
113	Computational Studies on Non-covalent Interactions of Carbon and Boron Fullerenes with Graphene. <i>ChemPhysChem</i> , 2013, 14, 1844-1852.	1.0	25
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	Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe <sub>2</sub> . <i>Applied Physics Letters</i> , 2016, 109, .	1.5	25
116	Theory of High Bias Coulomb Blockade in Ultrashort Molecules. <i>IEEE Nanotechnology Magazine</i> , 2007, 6, 536-544.	1.1	24
117	Clean WS <sub>2</sub> and MoS <sub>2</sub> Nanoribbons Generated by Laser-Induced Unzipping of the Nanotubes. <i>Small</i> , 2015, 11, 3916-3920.	5.2	24
118	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
119	Structure and electronic properties of the Watson-Crick base pairs: Role of hydrogen bonding. <i>Synthetic Metals</i> , 2005, 155, 398-401.	2.1	23
120	Aromatic Superclusters from All-Metal Aromatic and Antiaromatic Monomers, [Al <sub>4</sub> ] <sub>2</sub> - and [Al <sub>4</sub> ] <sub>4</sub> . <i>Journal of Physical Chemistry B</i> , 2006, 110, 20098-20101.	1.2	23
121	Line defects at the heterojunction of hybrid boron nitride-graphene nanoribbons. <i>Journal of Materials Chemistry C</i> , 2014, 2, 392-398.	2.7	23
122	Theoretical understanding of two-photon-induced fluorescence of isomorphous nucleoside analogs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10053-10058.	1.3	23
123	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
124	Tuning of hyperpolarizability, and one- and two-photon absorption of donor-acceptor and donor-acceptor-acceptor-type intramolecular charge transfer-based sensors. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17343-17355.	1.3	23
125	Synthesis, structure and magnetic properties of an inorganic-organic hybrid compound. <i>Journal of Materials Chemistry</i> , 2007, 17, 980-985.	6.7	22
126	One-dimensional organometallic anthracene wire and its N analogue: efficient half-metallic spin filters. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6924.	1.3	22



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127	Electronic and Magnetic Properties of Zigzag Boron-Nitride Nanoribbons with Even and Odd-Line Stone-Wales (5 <sup>+</sup> 7 <sup>-</sup> Pair) Defects. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3580-3594.	1.5	22
128	Imidazolyl $\pi$ -Naphthalenediimide $\pi$ -Based Threading Intercalators of DNA. <i>ChemBioChem</i> , 2016, 17, 2162-2171.	1.3	22
129	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
130	Exciton binding energy in the strong correlation limit of conjugated chains. <i>Physical Review B</i> , 1998, 58, 15329-15332.	1.1	21
131	Comparative study of electron conduction in azulene and naphthalene. <i>Bulletin of Materials Science</i> , 2008, 31, 353-358.	0.8	21
132	Spin-crossover molecule based thermoelectric junction. <i>Applied Physics Letters</i> , 2015, 106, .	1.5	21
133	Optical Unzipping of Carbon Nanotubes in Liquid Media. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16985-16993.	1.5	21
134	Mechanistic Insights into Hydrogen Activation by Frustrated N/Sn Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 2575-2579.	1.7	21
135	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
136	Odd $\sim$ Even Oscillations in First Hyperpolarizability of Dipolar Chromophores: A Role of Conformations of Spacers. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4112-4117.	1.1	20
137	Fluctuations at the Base Pair Level Effecting Charge Transfer in DNA. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3955-3962.	1.1	20
138	Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14754-14759.	1.2	20
139	Computational studies on structural and optical properties of single-stranded DNA encapsulated silver/gold clusters. <i>Journal of Materials Chemistry</i> , 2012, 22, 6774.	6.7	20
140	Enhancing Selectivity and Kinetics in Oxidative Photocyclization by Supramolecular Control. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13662-13665.	7.2	20
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