

# Swapan K Pati

## List of Publications by Year in descending order

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264  
papers

10,547  
citations

34105  
52  
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45317  
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. Angewandte Chemie - International Edition, 2010, 49, 4059-4062.	13.8	1,417
2	Novel properties of graphene nanoribbons: a review. Journal of Materials Chemistry, 2010, 20, 8207.	6.7	369
3	Uptake of H <sub>2</sub> and CO <sub>2</sub> by Graphene. Journal of Physical Chemistry C, 2008, 112, 15704-15707.	3.1	288
4	A study of graphene decorated with metal nanoparticles. Chemical Physics Letters, 2010, 497, 70-75.	2.6	286
5	Dipolar interactions and hydrogen bonding in supramolecular aggregates: understanding cooperative phenomena for 1st hyperpolarizability. Chemical Society Reviews, 2006, 35, 1305.	38.1	227
6	Density-matrix renormalization-group studies of the spin-1/2 Heisenberg system with dimerization and frustration. Physical Review B, 1995, 52, 6581-6587.	3.2	215
7	Half-Metallicity in Undoped and Boron Doped Graphene Nanoribbons in the Presence of Semilocal Exchange-Correlation Interactions. Journal of Physical Chemistry B, 2008, 112, 1333-1335.	2.6	188
8	Low-lying excited states and low-temperature properties of an alternating spin-1/2 chain: A density-matrix renormalization-group study. Physical Review B, 1997, 55, 8894-8904.	3.2	180
9	Visible-Near-Infrared and Fluorescent Copper Sensors Based on Julolidine Conjugates: Selective Detection and Fluorescence Imaging in Living Cells. Chemistry - A European Journal, 2011, 17, 11152-11161.	3.3	173
10	Light-Harvesting Supramolecular Phosphors: Highly Efficient Room Temperature Phosphorescence in Solution and Hydrogels. Angewandte Chemie - International Edition, 2021, 60, 19720-19724.	13.8	135
11	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
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. ACS Applied Materials & Interfaces, 2017, 9, 10664-10672.	8.0	118
13	Dipole orientation effects on nonlinear optical properties of organic molecular aggregates. Journal of Chemical Physics, 2003, 118, 8420-8427.	3.0	117
14	Alternating Spin and Orbital Dimerization and Spin-Gap Formation in Coupled Spin-Orbital Systems. Physical Review Letters, 1998, 81, 5406-5409.	7.8	112
15	Aqueous Phase Phosphorescence: Ambient Triplet Harvesting of Purely Organic Phosphors via Supramolecular Scaffolding. Angewandte Chemie - International Edition, 2018, 57, 17115-17119.	13.8	101
16	Conformationally Tuned Large Two-Photon Absorption Cross Sections in Simple Molecular Chromophores. Journal of the American Chemical Society, 2001, 123, 7287-7291.	13.7	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. Journal of Physical Chemistry C, 2011, 115, 10842-10850.	3.1	97
18	Transition Metal Embedded Two-Dimensional C <sub>3</sub> N <sub>4</sub> -Graphene Nanocomposite: A Multifunctional Material. Journal of Physical Chemistry C, 2014, 118, 15487-15494.	3.1	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.	13.8	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.	6.8	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.	3.0	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.	3.1	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.	10.3	77
25	Symmetrized density-matrix renormalization-group method for excited states of Hubbard models. <i>Physical Review B</i> , 1996, 54, 7598-7601.	3.2	74
26	Interaction of Inorganic Nanoparticles with Graphene. <i>ChemPhysChem</i> , 2011, 12, 937-943.	2.1	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.	2.8	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.	17.4	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.	10.3	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>Journal of Chemical Physics</i> , 2007, 126, 014701.	2.5	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.	3.1	68
32	High Capacity and High-Rate NASICON-Na <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.	19.5	68
33	Comparing the electron and hole mobilities in the $\hat{1}\pm$ and $\hat{1}^2$ phases of perylene: role of $\pi$ -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.	4.0	67
35	Competing Magnetic Interactions in a Dinuclear Ni(II) Complex: An Antiferromagnetic O <sup>2-</sup> -H <sup>+</sup> -O Moiety and Ferromagnetic N <sub>3</sub> -Ligand. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12-15.	2.6	66
36	Molecular Electronics: Effect of External Electric Field. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14718-14730.	3.1	66

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37	Toward DNA Conductivity: A Theoretical Perspective. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1881-1894.	4.6	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.	14.5	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.	5.6	65
40	Ambipolar Charge Transport in Î±-Oligofurans: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20436-20442.	3.1	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.	3.6	64
42	Arsenene nanosheets and nanodots. <i>New Journal of Chemistry</i> , 2018, 42, 14091-14095.	2.8	62
43	Conformational Tuning of Magnetic Interactions in Metal-DNA Complexes. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4977-4981.	13.8	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.	17.4	59
45	Alpha Lead Oxide (Î±PbO): A New 2D Material with Visible Light Sensitivity. <i>Small</i> , 2018, 14, e1703346.	10.0	58
46	N-Heterocyclic Germylene and Stannylene Catalyzed Cyanosilylation and Hydroboration of Aldehydes. <i>Organometallics</i> , 2019, 38, 1429-1435.	2.3	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.	13.7	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.	3.9	55
49	Magnetization properties of some quantum spin ladders. <i>Physical Review B</i> , 1999, 59, 396-410.	3.2	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.	3.3	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.	5.3	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.	3.1	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.	3.1	52

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55	Large carrier mobilities in octathio[8]circulene crystals: a theoretical study. Journal of Materials Chemistry, 2009, 19, 4356.	6.7	51
56	Aggregates of quadrupolar dyes for two-photon absorption: the role of intermolecular interactions. Physical Chemistry Chemical Physics, 2016, 18, 28198-28208.	2.8	51
57	Regulating Charge-Transfer in Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. Chemistry - A European Journal, 2019, 25, 3867-3874.	3.3	51
58	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
59	Nonlocal Electronic Distribution in Metallic Clusters: A Critical Examination of Aromatic Stabilization. Accounts of Chemical Research, 2007, 40, 213-221.	15.6	49
60	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
61	Dynamical nonlinear optical coefficients from the symmetrized density-matrix renormalization-group method. Physical Review B, 1999, 59, 14827-14830.	3.2	47
62	Computational Design of High Hydrogen Adsorption Efficiency in Molecular -Sulflower-. Journal of Physical Chemistry C, 2007, 111, 4487-4490.	3.1	47
63	Vanadium-Benzimidazole-Modified sDNA: A One-Dimensional Half-Metallic Ferromagnet. Journal of Physical Chemistry B, 2007, 111, 13877-13880.	2.6	46
64	Theoretical understanding of single-stranded DNA assisted dispersion of graphene. Journal of Materials Chemistry B, 2013, 1, 91-100.	5.8	46
65	Anion-Induced Room Temperature Phosphorescence from Emissive Charge-Transfer States. Journal of the American Chemical Society, 2022, 144, 10854-10861.	13.7	46
66	A density matrix renormalization group study of low-energy excitations and low-temperature properties of alternating spin systems. Journal of Physics Condensed Matter, 1997, 9, 8707-8726.	1.8	45
67	Binding energy of singlet excitons in the one-dimensional extended Hubbard-Peierls model. Physical Review B, 1997, 55, 15368-15371.	3.2	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. Inorganic Chemistry, 2016, 55, 6323-6331.	4.0	45
69	Edge reconstructions induce magnetic and metallic behavior in zigzag graphene nanoribbons. Carbon, 2010, 48, 4409-4413.	10.3	44
70	Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al <sup>3+</sup> Sensing. Crystal Growth and Design, 2016, 16, 82-91.	3.0	44
71	Effects of Dipole Orientations on Nonlinear Optical Properties of Oxo-Bridged Dinitroaniline Systems. Journal of Physical Chemistry A, 2004, 108, 320-325.	2.5	43
72	Quantum-confinement effects on the ordering of the lowest-lying excited states in conjugated chains. Physical Review B, 1997, 56, 9298-9301.	3.2	42

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73	Ring currents in condensed ring systems. International Journal of Quantum Chemistry, 1998, 70, 503-513.	2.0	42
74	Inorganic-Organic Hybrid Compounds: A Synthesis, Structure, and Magnetic Properties of the First Organically Templated Iron Oxalate-Phosphite, [C <sub>4</sub> N <sub>2</sub> H <sub>12</sub> ][Fe <sub>4</sub> (HPO <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> ], Possessing Infinite Fe-O-Fe Chains. Chemistry of Materials, 2005, 17, 2912-2917.	6.7	42
75	The First One-Dimensional Iron Phosphite-Phosphate, [Fe <sup>III</sup> (2,2'-bipyridine)(HPO <sub>3</sub> )(H <sub>2</sub> PO <sub>4</sub> )]: A Synthesis, Structure, and Magnetic Properties. Chemistry of Materials, 2005, 17, 638-643.	6.7	41
76	Role of Triple Bond in 1,2-Diphenylacetylene Crystal: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 24674-24677.	2.6	41
77	Anodic performance of black phosphorus in magnesium-ion batteries: the significance of Mg-P bond-synergy. Chemical Communications, 2016, 52, 8381-8384.	4.1	40
78	Thieno Analogues of RNA Nucleosides: A Detailed Theoretical Study. Journal of Physical Chemistry B, 2012, 116, 7618-7626.	2.6	39
79	Unique Approach to Copper(I) Silylene Chalcogenone Complexes. Inorganic Chemistry, 2017, 56, 1706-1712.	4.0	39
80	Doping Phosphorene with Holes and Electrons through Molecular Charge Transfer. ChemPhysChem, 2017, 18, 2985-2989.	2.1	37
81	Discordant Gd and Electronic Band Flattening Synergistically Induce High Thermoelectric Performance in n-type PbTe. ACS Energy Letters, 0, , 1625-1632.	17.4	37
82	Structures of Nucleobases Trapped within Au Triangles and Its Effects on Hydrogen Bonding in Base Pairs of DNA. Journal of Physical Chemistry B, 2006, 110, 18661-18664.	2.6	36
83	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
84	Nonlinear Optical Properties in Calix[n]arenes: Orientation Effects of Monomers. Chemistry - A European Journal, 2005, 11, 4961-4969.	3.3	35
85	Sequence Dependent Electron Transport in Wet DNA: Ab Initio and Molecular Dynamics Studies. Physical Review Letters, 2008, 101, 176805.	7.8	35
86	On Nitrogen Insertion of a Diazo Compound into a Germanium(II) Hydrogen Bond and a Comparable Reaction with Diethyl Azodicarboxylate. Angewandte Chemie - International Edition, 2009, 48, 4246-4248.	13.8	35
87	BN-decorated graphene nanoflakes with tunable opto-electronic and charge transport properties. Journal of Materials Chemistry C, 2014, 2, 2918-2928.	5.5	35
88	On the Mechanism of Frustrated Lewis Pair Catalysed Hydrogenation of Carbonyl Compounds. Chemistry - A European Journal, 2017, 23, 1078-1085.	3.3	35
89	Observation of tango-like chains in a one-dimensional metal-organic polymer. Journal of Materials Chemistry, 2003, 13, 2937-2941.	6.7	34
90	Doping single-walled carbon nanotubes through molecular charge-transfer: a theoretical study. Nanoscale, 2010, 2, 1190.	5.6	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.	2.8	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.	3.3	34
93	The interaction of halogen molecules with SWNTs and graphene. <i>RSC Advances</i> , 2012, 2, 1181-1188.	3.6	33
94	Phase Transition of MoS <sub>2</sub> Bilayer Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3776-3780.	3.1	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.	2.8	33
96	Chiral Arylene Diimide Phosphors: Circularly Polarized Ambient Phosphorescence from Bischromophoric Pyromellitic Diimides. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	33
97	Aromaticity in Stable Tiara Nickel Thiolates: Computational and Structural Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11647-11649.	2.5	32
98	Current-voltage characteristics in donor-acceptor systems: Implications of a spatially varying electric field. <i>Physical Review B</i> , 2005, 72, .	3.2	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.	1.8	31
100	Laser Shock Tuning Dynamic Interlayer Coupling in Graphene-Boron Nitride Moiré Superlattices. <i>Nano Letters</i> , 2019, 19, 283-291.	9.1	31
101	Magnetic Interactions in Layered Nickel Alkanethiolates. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1868-1870.	3.1	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.	2.6	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.	3.0	28
105	Cobalt-Based Coordination Polymer for Oxygen Reduction Reaction. <i>ACS Omega</i> , 2018, 3, 3830-3834.	3.5	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.	3.0	27
107	Functional Corannulene: Diverse Structures, Enhanced Charge Transport, and Tunable Optoelectronic Properties. <i>ChemPhysChem</i> , 2014, 15, 885-893.	2.1	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.	3.0	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.	3.2	25
110	Rationalization of the $\pi$ - $\pi^*$ (Anti)aromaticity in All Metal Molecular Clusters. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 824-826.	5.3	25
111	Structure and Transport Characteristics of Modified DNA with Magnetic Ions. <i>Physical Review Letters</i> , 2007, 98, 136601.	7.8	25
112	Molecular Architectonics of Stereochemically Constrained $\pi$ - $\pi^*$ Complementary Functional Modules. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5838-5847.	2.4	25
113	Computational Studies on Non-covalent Interactions of Carbon and Boron Fullerenes with Graphene. <i>ChemPhysChem</i> , 2013, 14, 1844-1852.	2.1	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.	2.6	25
115	Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe <sub>2</sub> . <i>Applied Physics Letters</i> , 2016, 109, .	3.3	25
116	Theory of High Bias Coulomb Blockade in Ultrashort Molecules. <i>IEEE Nanotechnology Magazine</i> , 2007, 6, 536-544.	2.0	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.	10.0	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.	10.3	24
119	Structure and electronic properties of the Watson-Crick base pairs: Role of hydrogen bonding. <i>Synthetic Metals</i> , 2005, 155, 398-401.	3.9	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.	2.6	23
121	Line defects at the heterojunction of hybrid boron nitride-graphene nanoribbons. <i>Journal of Materials Chemistry C</i> , 2014, 2, 392-398.	5.5	23
122	Theoretical understanding of two-photon-induced fluorescence of isomorphous nucleoside analogs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10053-10058.	2.8	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.	3.1	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.	2.8	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 $\pi$ -anthracene wire and its $\pi$ -N analogue: efficient half-metallic spin filters. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6924.	2.8	22



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127	Electronic and Magnetic Properties of Zigzag Boron-Nitride Nanoribbons with Even and Odd-Line Stone-Wales (5â€”7 Pair) Defects. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3580-3594.	3.1	22
128	Imidazolylâ€”Naphthalenediimideâ€”Based Threading Intercalators of DNA. <i>ChemBioChem</i> , 2016, 17, 2162-2171.	2.6	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.	4.6	22
130	Exciton binding energy in the strong correlation limit of conjugated chains. <i>Physical Review B</i> , 1998, 58, 15329-15332.	3.2	21
131	Comparative study of electron conduction in azulene and naphthalene. <i>Bulletin of Materials Science</i> , 2008, 31, 353-358.	1.7	21
132	Spin-crossover molecule based thermoelectric junction. <i>Applied Physics Letters</i> , 2015, 106, .	3.3	21
133	Optical Unzipping of Carbon Nanotubes in Liquid Media. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16985-16993.	3.1	21
134	Mechanistic Insights into Hydrogen Activation by Frustrated N/Sn Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 2575-2579.	3.3	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.	2.6	21
136	Oddâ”Even Oscillations in First Hyperpolarizability of Dipolar Chromophores:â”Role of Conformations of Spacers. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4112-4117.	2.5	20
137	Fluctuations at the Base Pair Level Effecting Charge Transfer in DNA. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3955-3962.	2.5	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.	2.6	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.	13.8	20
141	Linear and nonlinear optical polarizabilities in supramolecular aggregates: Effects of hydrogen bonding and dipolar interactions. <i>Computational and Theoretical Chemistry</i> , 2005, 756, 97-102.	1.5	19
142	Structural, electronic and photophysical properties of analogous RNA nucleosides: a theoretical study. <i>New Journal of Chemistry</i> , 2013, 37, 3640.	2.8	19
143	Transport in molecular wire with long-range Coulomb interactions: A mean-field approach. <i>Journal of Chemical Physics</i> , 2003, 118, 6529-6535.	3.0	18
144	Beyond the FÃ¶rster formulation for resonance energy transfer: the role of dark states. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12734.	2.8	18

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145	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
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