Ayan Datta

List of Publications by Year in descending order

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232 papers	7,232 citations	57719 44 h-index	95218 68 g-index
240 all docs	240 docs citations	240 times ranked	7796 citing authors

#	Article	IF	Citations
1	Substituent effect of benzyl moiety in nitroquinoxaline small molecules upon DNA binding: Cumulative destacking of DNA nucleobases leading to histone eviction. European Journal of Medicinal Chemistry, 2022, 229, 113995.	2.6	2
2	Stereoelectronic and dynamical effects dictate nitrogen inversion during valence isomerism in benzene imine. Chemical Science, 2022, 13, 704-712.	3.7	5
3	Stable room temperature ferroelectricity in hydrogen-bonded supramolecular assemblies of ambipolar Ï€-systems. Chemical Science, 2022, 13, 781-788.	3.7	14
4	Remarkable CO_x tolerance of Ni³⁺ active species in a Ni₂O₃ catalyst for sustained electrochemical urea oxidation. Journal of Materials Chemistry A, 2022, 10, 4209-4221.	5.2	57
5	Metalâ€free Kinugasa reaction catalyzed by external electric field. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	8
6	A Hierarchical (Macro)molecular Assembly Assisted by Donorâ€“Acceptor Chargeâ€Transfer Interactions Exhibiting Roomâ€Temperature Ferroelectricity. Angewandte Chemie - International Edition, 2022, 61, .	7.2	13
7	Adsorbate-Induced Phase Transformation of Ambient Stable Noncubic Lattices in Au Microcrystallites. Journal of Physical Chemistry C, 2022, 126, 823-831.	1.5	3
8	Deciphering the Role of Substitution in Transitionâ€Metal Phosphorous Trisulfide (100) Surface: A Highly Efficient and Durable Ptâ€free ORR Electrocatalyst. ChemPhysChem, 2022, 23, .	1.0	1
9	Epitaxial Orientation Angle Tuned Disk-on-Rod Nanoheterostructures for Boosting Charge Transfer. Journal of Physical Chemistry Letters, 2022, 13, 3804-3811.	2.1	2
10	Thiazole Containing PNA Mimic Regulates c-MYC Gene Expression through DNA G-Quadruplex. Bioconjugate Chemistry, 2022, 33, 1145-1155.	1.8	2
11	Rational Design of Biaxial Tensile Strain for Boosting Electronic and Ionic Conductivities of Na ₂ MnSiO ₄ for Rechargeable Sodiumâ€ion Batteries. ChemistryOpen, 2022, 11, .	0.9	3
12	Compression Produces a Square-Planar Iron Tetracarbonyl. Inorganic Chemistry, 2022, 61, 9055-9062.	1.9	1
13	Performance of the nitrogen reduction reaction on metal bound g-C₆N₆: a combined approach of machine learning and DFT. Physical Chemistry Chemical Physics, 2022, 24, 17050-17058.	1.3	15
14	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp²)â€“H Activation in Conformationally Flexible Arylammonium Salts. Journal of Organic Chemistry, 2022, 87, 9222-9231.	1.7	2
15	Designing C₆N₆/C₂N van der Waals heterostructures for photogenerated charge carrier separation. Physical Chemistry Chemical Physics, 2021, 23, 3925-3933.	1.3	25
16	Molecular Mechanism for the Self-Supported Synthesis of Graphitic Carbon Nitride from Urea Pyrolysis. Journal of Physical Chemistry Letters, 2021, 12, 1396-1406.	2.1	20
17	Evolutionary structure prediction-assisted design of anode materials for Ca-ion battery based on phosphorene. Physical Chemistry Chemical Physics, 2021, 23, 9466-9475.	1.3	13
18	Prolinamide plays a key role in promoting copper-catalyzed cycloaddition of azides and alkynes in aqueous media via unprecedented metallacycle intermediates. Organic Chemistry Frontiers, 2021, 8, 2434-2441.	2.3	5

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19	Nickelâ€“cobalt oxalate as an efficient non-precious electrocatalyst for an improved alkaline oxygen evolution reaction. Nanoscale Advances, 2021, 3, 3770-3779.	2.2	19
20	Tuning of the optoelectronic properties of peptide-appended core-substituted naphthalenediimides: the role of self-assembly of two positional isomers. Soft Matter, 2021, 17, 7168-7176.	1.2	9
21	Tuning intermediate adsorption in structurally ordered substituted PdCu3 intermetallic nanoparticles for enhanced ethanol oxidation reaction. Chemical Communications, 2021, 57, 4508-4511.	2.2	9
22	Unveiling the Excellent Electrocatalytic Activity of Grain-Boundary Enriched Anisotropic Pure Gold Nanostructures toward Hydrogen Evolution Reaction: A Combined Approach of Experiment and Theory. ACS Applied Energy Materials, 2021, 4, 3017-3032.	2.5	9
23	Molecular Dynamics Simulations Reveal Orientation-Dependent Nanotoxicity of Black Phosphorene toward Dimeric Proteins. ACS Applied Nano Materials, 2021, 4, 3095-3107.	2.4	15
24	Novel Tetradentate Phosphonate Ligand Based Bioinspired Co-Metalâ€“Organic Frameworks: Robust Electrocatalyst for the Hydrogen Evolution Reaction in Different Mediums. Crystal Growth and Design, 2021, 21, 2614-2623.	1.4	17
25	Formation of Metallic Polyferrocene Chains under Pressure. Journal of Physical Chemistry A, 2021, 125, 3362-3368.	1.1	6
26	Synthetic and Computational Studies on Rh^{III}-Catalyzed Redox-Neutral Cascade of Carbenoid Functionalization and Dephosphonylative Annulation. Journal of Organic Chemistry, 2021, 86, 7069-7077.	1.7	13
27	An NHCâ€Stabilised Phosphinidene for Catalytic Formylation: A DFTâ€Guided Approach. Chemistry - A European Journal, 2021, 27, 11656-11662.	1.7	6
28	Direct CO₂ capture and conversion to fuels on magnesium nanoparticles under ambient conditions simply using water. Chemical Science, 2021, 12, 5774-5786.	3.7	25
29	Harnessing Noncovalent Interactions for a Directed Evolution of a Six-Component Molecular Crystal. Journal of Physical Chemistry B, 2021, 125, 12584-12591.	1.2	6
30	Goldâ€Catalyzed Crossâ€Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. Chemistry - A European Journal, 2020, 26, 1442-1487.	1.7	128
31	Screening two dimensional materials for the transportation and delivery of diverse genetic materials. Nanoscale, 2020, 12, 703-719.	2.8	23
32	Harnessing the Efficacy of 2-Pyridone Ligands for Pd-Catalyzed (Î²/Î³)-C(sp³)â€“H Activations. Journal of Organic Chemistry, 2020, 85, 13228-13238.	1.7	22
33	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. Journal of Physical Chemistry C, 2020, 124, 24451-24459.	1.5	13
34	Cobalt phthalocyanine (CoPc) monolayer: A computational study on oxygen reduction reaction (ORR). AIP Conference Proceedings, 2020, , .	0.3	0
35	Molecular designs for expanding the limits of ultralong Câ€“C bonds and ultrashort Hâ‹¯H non-bonded contacts. Chemical Communications, 2020, 56, 15377-15386.	2.2	12
36	Heavy-atom tunneling in organic transformations. Journal of Chemical Sciences, 2020, 132, 1.	0.7	8

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37	Deoxygenation of nitrosoarene by N-heterocyclic carbene (NHC): an elusive Breslow-type intermediate bridging carbene and nitrene. Chemical Communications, 2020, 56, 12166-12169.	2.2	2
38	Paradoxical design of a serendipitous pyrazolate bridging mode: a pragmatic strategy for inducing ineluctable ferromagnetic coupling. Dalton Transactions, 2020, 49, 13704-13716.	1.6	2
39	Disentangling the liquid phase exfoliation of two-dimensional materials: an â€œin silicoâ€• perspective. Physical Chemistry Chemical Physics, 2020, 22, 22157-22179.	1.3	17
40	Polymorphism Dependent 9-Phosphoanthracene Derivative Exhibiting Thermally Activated Delayed Fluorescence: A Computational Investigation. Journal of Physical Chemistry A, 2020, 124, 11025-11037.	1.1	17
41	Enhanced Photophysical Properties of Bi2S3/AgBiS2 Nanoheterostructures Synthesized via Ag(I) Cation Exchange-Mediated Transformation of Binary Bi2S3. Journal of Physical Chemistry C, 2020, 124, 12824-12833.	1.5	5
42	Transitionâ€Metal Phosphorus Trisulfides and its Vacancy Defects: Emergence of a New Class of Anode Material for Liâ€Ion Batteries. ChemSusChem, 2020, 13, 3855-3864.	3.6	30
43	Delicate Balance of Nonâ€Covalent Forces Govern the Biocompatibility of Graphitic Carbon Nitride towards Genetic Materials. ChemPhysChem, 2020, 21, 1836-1846.	1.0	12
44	Defects in nanosilica catalytically convert CO ₂ to methane without any metal and ligand. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6383-6390.	3.3	68
45	Frontispiece: Goldâ€Catalyzed Crossâ€Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. Chemistry - A European Journal, 2020, 26, .	1.7	1
46	Transition-State-like Planar Structures for Amine Inversion with Ultralong Câ€“C Bonds in Diamino-o-carborane and Diamino-o-dodecahedron. Journal of the American Chemical Society, 2020, 142, 5331-5337.	6.6	18
47	Enhancement in electrical conductivity of a porous indium based metalâ€“organic framework upon I₂ uptake: combined experimental and theoretical investigations. Journal of Materials Chemistry C, 2020, 8, 4836-4842.	2.7	13
48	A Thiadiazole-Based Covalent Organic Framework: A Metal-Free Electrocatalyst toward Oxygen Evolution Reaction. ACS Catalysis, 2020, 10, 5623-5630.	5.5	140
49	Remote Functionalization through Symmetric or Asymmetric Substitutions Control the Pathway of Intermolecular Singlet Fission. Journal of Chemical Theory and Computation, 2019, 15, 5014-5023.	2.3	9
50	Hierarchical Noncovalent Interactions between Molecules Stabilize Multicomponent Cocrystals. Crystal Growth and Design, 2019, 19, 4802-4809.	1.4	14
51	Pt/Co₃O₄ Surpasses Benchmark Pt/C: An Approach Toward Next Generation Hydrogen Evolution Electrocatalyst. ACS Applied Energy Materials, 2019, 2, 5613-5621.	2.5	29
52	RuIII(edta)-mediated interaction of nitrite and sulphide: formation of an N-bonded thionitrous acid (HSNO) complex of RuIII(edta) in aqueous solution. New Journal of Chemistry, 2019, 43, 15311-15315.	1.4	3
53	Influence of Axial Linkers on Polymerization in Paddle-Wheel Cu(II) Coordination Polymers for the Application of Optoelectronics Devices. Crystal Growth and Design, 2019, 19, 6283-6290.	1.4	20
54	Transforming atmospheric CO₂ into alternative fuels: a metal-free approach under ambient conditions. Chemical Science, 2019, 10, 1879-1884.	3.7	19

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55	Aryl-platform-based tetrapodal 2-iodo-imidazolium as an excellent halogen bond receptor in aqueous medium. Chemical Communications, 2019, 55, 1506-1509.	2.2	22
56	Topological Phase Transition in Sb₂Mg₃ Assisted by Strain. ACS Omega, 2019, 4, 8701-8706.	1.6	11
57	Visible light driven efficient metal free single atom catalyst supported on nanoporous carbon nitride for nitrogen fixation. Physical Chemistry Chemical Physics, 2019, 21, 12346-12352.	1.3	64
58	Computationally Driven Design Principles for Singlet Fission in Organic Chromophores. Journal of Physical Chemistry C, 2019, 123, 19257-19268.	1.5	22
59	A Solution Processed Ultrathin Molecular Dielectric for Organic Field-Effect Transistors. ACS Applied Electronic Materials, 2019, 1, 485-493.	2.0	4
60	Analysis of pseudo jahnâ€“teller distortion based on natural bond orbital theory: Case study for silicene. Journal of Computational Chemistry, 2019, 40, 1488-1495.	1.5	14
61	Aggregation induced non-emissive-to-emissive switching of molecular platinum clusters. Nanoscale, 2019, 11, 5914-5919.	2.8	13
62	Intramolecular Singlet Fission in Quinoidal Dihydrothiophene. Journal of Physical Chemistry C, 2019, 123, 4749-4754.	1.5	10
63	Interaction of a bioactive molecule with surfaces of nanoscale transition metal oxides: experimental and theoretical studies. New Journal of Chemistry, 2019, 43, 16621-16628.	1.4	4
64	Red-Emitting Copper Nanoclusters: From Bulk-Scale Synthesis to Catalytic Reduction. ACS Sustainable Chemistry and Engineering, 2019, 7, 1998-2007.	3.2	46
65	Gauging the Nanotoxicity of h2D-C₂N toward Single-Stranded DNA: An in Silico Molecular Simulation Approach. ACS Applied Materials & Interfaces, 2018, 10, 13805-13818.	4.0	39
66	Controlled Pore Sizes in Monolayer C₂N Act as Ultrasensitive Probes for Detection of Gaseous Pollutants (HF, HCN, and H₂S). Journal of Physical Chemistry C, 2018, 122, 2248-2258.	1.5	53
67	Dynamical Effects along the Bifurcation Pathway Control Semibullvalene Formation in Deazetization Reactions. Journal of Physical Chemistry B, 2018, 122, 1239-1244.	1.2	14
68	Topological Insulator in Two-Dimensional SiGe Induced by Biaxial Tensile Strain. ACS Omega, 2018, 3, 1-7.	1.6	23
69	Novel Brâ‹…â‹…â‹…Ï€(Chelate) Interaction in a 1D Coordination Polymer Revealing Aromaticity. ChemistrySelect, 2018, 3, 4289-4291.	0.7	18
70	Evidence of homo-FRET in quantum dotâ€“dye heterostructured assembly. Physical Chemistry Chemical Physics, 2018, 20, 9523-9535.	1.3	23
71	Ultrafast Relaxation Dynamics of Luminescent Copper Nanoclusters (Cu₇L₃) and Efficient Electron Transfer to Functionalized Reduced Graphene Oxide. Journal of Physical Chemistry C, 2018, 122, 13354-13362.	1.5	44
72	Structure and Electronic Properties of Unnatural Base Pairs: The Role of Dispersion Interactions. ChemPhysChem, 2018, 19, 67-74.	1.0	16

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73	A Vision on Organosilicon Chemistry and Silicene. Nanoscience and Technology, 2018, , 1-21.	1.5	2
74	Silicon-Doped Nitrogen-Coordinated Graphene as Electrocatalyst for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 27233-27240.	1.5	59
75	Design Rules for the Generation of Stable Quartet Phases of Nucleobases over Two-Dimensional Materials. Journal of Physical Chemistry C, 2018, 122, 28918-28933.	1.5	26
76	Strain-Induced Topological Insulator in Methyl-Decorated SiGe Films. Journal of Physical Chemistry C, 2018, 122, 25127-25133.	1.5	12
77	Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. Inorganic Chemistry, 2018, 57, 11995-12009.	1.9	29
78	Doped boron nitride surfaces: potential metal free bifunctional catalysts for non-aqueous Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2018, 20, 16485-16492.	1.3	10
79	Reactive Molecular Dynamics Simulations of Self-Assembly of Polytwistane and Its Application for Nanofibers. Journal of Physical Chemistry C, 2018, 122, 19204-19211.	1.5	11
80	Gold(I)-Catalyzed Intramolecular Dielsâ€“Alder Reaction: Evolution of Trappable Intermediates via Asynchronous Transition States. Journal of Organic Chemistry, 2018, 83, 11167-11177.	1.7	19
81	Understanding Thermal and Photochemical Arylâ€“Aryl Crossâ€Coupling by the Au^I/Au^{III} Redox Couple. Chemistry - A European Journal, 2018, 24, 13636-13646.	1.7	21
82	Pseudo-Jahnâ€“Teller effects in two-dimensional silicene, germanene and stanene: a crystal orbital vibronic coupling density analysis. Bulletin of Materials Science, 2018, 41, 1.	0.8	5
83	An Azoaromatic Ligand as Four Electron Four Proton Reservoir: Catalytic Dehydrogenation of Alcohols by Its Zinc(II) Complex. Inorganic Chemistry, 2018, 57, 6816-6824.	1.9	45
84	Noble-Metal-Supported GeS Monolayer as Promising Single-Atom Catalyst for CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 14488-14498.	1.5	35
85	Phase Coexistence and Strain-Induced Topological Insulator in Two-Dimensional BiAs. Journal of Physical Chemistry C, 2018, 122, 15047-15054.	1.5	33
86	Tunneling Control: Competition between 6Ï€-Electrocyclization and [1,5]H-Sigmatropic Shift Reactions in Tetrahydro-1H-cyclobuta[e]indene Derivatives. Journal of Organic Chemistry, 2017, 82, 1558-1566.	1.7	23
87	Direct and Autocatalytic Reductive Elimination from Gold Complexes ([(Ph₃P)Au(Ar)(CF₃)(X)], X=F, Cl, Br, I): The Key Role of Halide Ligands. Chemistry - A European Journal, 2017, 23, 4169-4179.	1.7	31
88	Polymorphism Controlled Singlet Fission in TIPS-Anthracene: Role of Stacking Orientation. Journal of Physical Chemistry C, 2017, 121, 1412-1420.	1.5	60
89	Size specific emission in peptide capped gold quantum clusters with tunable photoswitching behavior. Nanoscale, 2017, 9, 4419-4429.	2.8	32
90	Ordering and Dynamics for the Formation of Two-Dimensional Molecular Crystals on Black Phosphorene. Journal of Physical Chemistry C, 2017, 121, 10210-10223.	1.5	43

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91	Exotic Physics and Chemistry of Two-Dimensional Phosphorus: Phosphorene. Journal of Physical Chemistry Letters, 2017, 8, 2909-2916.	2.1	71
92	Theoretical study of Au 4 thymine, Au 20 and Ag 20 uracil and thymine complexes for surface enhanced Raman scattering. Computational and Theoretical Chemistry, 2017, 1111, 1-13.	1.1	15
93	Monolayer Group IVâ€“VI Monochalcogenides: Low-Dimensional Materials for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2017, 121, 7615-7624.	1.5	154
94	Design of van der Waals Two-Dimensional Heterostructures from Facially Polarized Janus All-Cis 1,2,3,4,5,6-Hexafluorocyclohexane (C6H6F6). Journal of Physical Chemistry C, 2017, 121, 1752-1762.	1.5	18
95	Exploring Ultrashort Hydrogenâ€“Hydrogen Nonbonded Contacts in Constrained Molecular Cavities. Journal of Physical Chemistry B, 2017, 121, 825-834.	1.2	23
96	Deciphering the Role of Solvents in the Liquid Phase Exfoliation of Hexagonal Boron Nitride: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2017, 121, 811-822.	1.5	59
97	Influence of Hofmeister I^{â€“} on Tuning Optoelectronic Properties of Ampholytic Polythiophene by Varying pH and Conjugating with RNA. Langmuir, 2017, 33, 12739-12749.	1.6	16
98	Role of Carbon Support for Subnanometer Gold-Cluster-Catalyzed Disiloxane Synthesis from Hydrosilane and Water. Journal of Physical Chemistry C, 2017, 121, 20101-20112.	1.5	9
99	Two-Dimensional Grapheneâ€“Gold Interfaces Serve as Robust Templates for Dielectric Capacitors. ACS Applied Materials & Interfaces, 2017, 9, 34213-34220.	4.0	28
100	Visibleâ€Lightâ€Mediated Excited State Relaxation in Semiâ€Synthetic Genetic Alphabet: d5SICS and dNaM. Chemistry - A European Journal, 2017, 23, 11494-11498.	1.7	16
101	Understanding the Reactivity of CO₃^{Â·â€“} and NO₂^{Â·} Radicals toward S-Containing and Aromatic Amino Acids. Journal of Physical Chemistry B, 2017, 121, 7621-7632.	1.2	10
102	Coexistence of Normal and Auxetic Behavior in a Thermally and Chemically Stable sp³ Nanothread: Poly[5]asterane. Chemistry - A European Journal, 2017, 23, 12917-12923.	1.7	12
103	External electric field control: driving the reactivity of metal-free azideâ€“alkyne click reactions. Physical Chemistry Chemical Physics, 2017, 19, 22482-22486.	1.3	47
104	Effect of Doping in Controlling the Structure, Reactivity, and Electronic Properties of Pristine and Ca(II)-Intercalated Layered Silicene. Journal of Physical Chemistry C, 2017, 121, 15169-15180.	1.5	17
105	Janus allâ€cisâ€1,2,3,4,5,6â€Hexafluorocyclohexane: A Molecular Motif for Aggregationâ€Induced Enhanced Polarization. ChemPhysChem, 2016, 17, 2373-2381.	1.0	29
106	Classroom. Resonance, 2016, 21, 377-379.	0.2	0
107	Controlling electronic effects and intermolecular packing in contorted polyaromatic hydrocarbons (c-PAHs): towards high mobility field effect transistors. Physical Chemistry Chemical Physics, 2016, 18, 14886-14893.	1.3	11
108	Supported Sub-Nanometer Gold Cluster Catalyzed Transfer Hydrogenation of Aldehydes to Alcohols. Journal of Physical Chemistry C, 2016, 120, 24449-24456.	1.5	14

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109	Exclusively Ligand-Mediated Catalytic Dehydrogenation of Alcohols. Inorganic Chemistry, 2016, 55, 9602-9610.	1.9	55
110	Nonequimolar Mixture of Organic Acids and Bases: An Exception to the Rule of Thumb for Salt or Cocrystal. Journal of Physical Chemistry B, 2016, 120, 7606-7613.	1.2	25
111	Metalâ€Free Reduction of CO₂ to Methoxyborane under Ambient Conditions through Borondiformate Formation. Angewandte Chemie - International Edition, 2016, 55, 15147-15151.	7.2	50
112	Steric and electric field driven distortions in aromatic molecules: spontaneous and non-spontaneous symmetry breaking. Physical Chemistry Chemical Physics, 2016, 18, 31160-31167.	1.3	23
113	Two-Dimensional Group IV Monochalcogenides: Anode Materials for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 14522-14530.	1.5	120
114	Capping Black Phosphorene by h-BN Enhances Performances in Anodes for Li and Na Ion Batteries. ACS Energy Letters, 2016, 1, 253-259.	8.8	126
115	Multifunctional mixed ligand metal organic frameworks: X-ray structure, adsorption, luminescence and electrical conductivity with theoretical correlation. CrystEngComm, 2016, 18, 5754-5763.	1.3	23
116	Role of Heavy Atom Tunneling in Myersâ€“Saito Cyclization of Cyclic Enyne-Cumulene Systems. Journal of Physical Chemistry B, 2016, 120, 945-950.	1.2	26
117	Dual Fluorescence in GFP Chromophore Analogues: Chemical Modulation of Charge Transfer and Proton Transfer Bands. Journal of Physical Chemistry B, 2016, 120, 3503-3510.	1.2	26
118	Pseudo-Jahnâ€“Teller Distortion in Two-Dimensional Phosphorus: Origin of Black and Blue Phases of Phosphorene and Band Gap Modulation by Molecular Charge Transfer. Journal of Physical Chemistry Letters, 2016, 7, 1288-1297.	2.1	73
119	Strain Control: Reversible H₂ Activation and H₂/D₂ Exchange in Pt Complexes. Inorganic Chemistry, 2016, 55, 3023-3029.	1.9	18
120	Pseudo Jahnâ€“Teller distortion for a tricyclic carbon sulfide (C6S8) and its suppression in S-oxygenated dithiine (C4H4(SO2)2). Chemical Physics, 2015, 460, 101-105.	0.9	27
121	Topochemical Transformations of CaX₂ (X=C, Si, Ge) to Form Freeâ€Standing Twoâ€Dimensional Materials. Chemistry - A European Journal, 2015, 21, 18454-18460.	1.7	31
122	Fluorescence from an H-aggregated naphthalenediimide based peptide: photophysical and computational investigation of this rare phenomenon. Physical Chemistry Chemical Physics, 2015, 17, 30398-30403.	1.3	40
123	Cooperativity in a New Role: Stabilization of the Ammonium Salts in the Solid State over Their H-Bonded Complexes in the Gas Phase. Journal of Physical Chemistry C, 2015, 119, 926-933.	1.5	14
124	Electronic and Chemical Properties of Germanene: The Crucial Role of Buckling. Journal of Physical Chemistry C, 2015, 119, 3802-3809.	1.5	125
125	1,4-Dithiineâ"Puckered in the Gas Phase but Planar in Crystals: Role of Cooperativity. Journal of Physical Chemistry C, 2015, 119, 15770-15776.	1.5	22
126	Half-sandwich Ru(Î·⁶-C₆H₆) complexes with chiral aroylthioureas for enhanced asymmetric transfer hydrogenation of ketones â€“ experimental and theoretical studies. Catalysis Science and Technology, 2015, 5, 4790-4799.	2.1	28

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127	What Sustains the Unnatural Base Pairs (UBPs) with No Hydrogen Bonds. Journal of Physical Chemistry B, 2015, 119, 5839-5845.	1.2	36
128	Mechanistic insights into the synergistic catalysis by Au(<scp>i</scp>), Ga(<scp>iii</scp>), and counterions in the Nakamura reaction. Organic and Biomolecular Chemistry, 2015, 13, 7412-7420.	1.5	28
129	Small Organic Molecules for Efficient Singlet Fission: Role of Silicon Substitution. Journal of Physical Chemistry C, 2015, 119, 25696-25702.	1.5	36
130	Metal Free Azideâ€“Alkyne Click Reaction: Role of Substituents and Heavy Atom Tunneling. Journal of Physical Chemistry B, 2015, 119, 11540-11547.	1.2	23
131	The role of N7 protonation of guanine in determining the structure, stability and function of RNA base pairs. Physical Chemistry Chemical Physics, 2015, 17, 26249-26263.	1.3	27
132	Preparation of multi-coloured different sized fluorescent gold clusters from blue to NIR, structural analysis of the blue emitting Au₇cluster, and cell-imaging by the NIR gold cluster. Nanoscale, 2015, 7, 1912-1920.	2.8	51
133	Understanding the Mechanisms of Unusually Fast Hï£¿H, Cï£¿H, and Cï£¿C Bond Reductive Eliminations from Gold(III) Complexes. Chemistry - A European Journal, 2014, 20, 14650-14658.	1.7	48
134	Influence of ring fusion stereochemistry on the stereochemical outcome in photo-induced Dielsâ€“Alder reaction of fused bicycloheptenone derivatives. Tetrahedron, 2014, 70, 9783-9790.	1.0	5
135	Phenalenyl in a Different Role: Catalytic Activation through the Nonbonding Molecular Orbital. ACS Catalysis, 2014, 4, 4307-4319.	5.5	40
136	Light Harvesting and Amplification of Emission of Donor Peryleneâ€“Acceptor Perylene Aggregates in Aqueous Medium. Chemistry - A European Journal, 2014, 20, 3019-3022.	1.7	13
137	Chargeâ€Transfer Complex Formation in Gelation: The Role of Solvent Molecules with Different Electronâ€Donating Capacities. Chemistry - A European Journal, 2014, 20, 5721-5726.	1.7	44
138	Design and Applications of Noncanonical DNA Base Pairs. Journal of Physical Chemistry Letters, 2014, 5, 154-166.	2.1	41
139	Structures and Chemical Properties of Silicene: Unlike Graphene. Accounts of Chemical Research, 2014, 47, 593-602.	7.6	291
140	Synthesis, structure, photocatalytic and magnetic properties of an oxo-bridged copper dimer. RSC Advances, 2014, 4, 21195-21200.	1.7	9
141	Tunneling Assists the 1,2â€Hydrogen Shift in Nâ€Heterocyclic Carbenes. Angewandte Chemie - International Edition, 2014, 53, 9587-9591.	7.2	36
142	Why Does Substitution of Thymine by 6-Ethynylpyridone Increase the Thermostability of DNA Double Helices?. Journal of Physical Chemistry B, 2014, 118, 6586-6596.	1.2	17
143	Tunnelling effects in chemistry. Resonance, 2014, 19, 160-174.	0.2	4
144	Role of Quantum Mechanical Tunneling on the Î³-Effect of Silicon on Carbenes in 3-Trimethylsilylcyclobutylidene. Journal of Physical Chemistry B, 2014, 118, 2553-2558.	1.2	16

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145	Color Polymorphism: Understanding the Diverse Solidâ€State Packing and Color in Dimethylâ€3,6â€dichloroâ€2,5â€dihydroxyterephthalate. Chemistry - A European Journal, 2014, 20, 3218-3224.	1.7	15
146	Structures and Electronic Properties of Heavier Congeners of Disk-Like Molecules: (Si, Ge) Sulflower and (Si, Ge) Olympicene. Journal of Physical Chemistry C, 2014, 118, 12115-12120.	1.5	25
147	Can Arsenates Replace Phosphates in Natural Biochemical Processes? A Computational Study. Journal of Physical Chemistry B, 2013, 117, 8340-8346.	1.2	27
148	Pronounced Tunneling Effect of Proton Transfer in Thiotropolone at Room Temperature: A Reply. Angewandte Chemie - International Edition, 2013, 52, 8206-8207.	7.2	5
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