

# Ayan Datta

## List of Publications by Year in descending order

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232  
papers

7,232  
citations

57758

44  
h-index

95266

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. <i>European Journal of Medicinal Chemistry</i> , 2022, 229, 113995.	5.5	2
2	Stereoelectronic and dynamical effects dictate nitrogen inversion during valence isomerism in benzene imine. <i>Chemical Science</i> , 2022, 13, 704-712.	7.4	5
3	Stable room temperature ferroelectricity in hydrogen-bonded supramolecular assemblies of ambipolar $\pi$ -systems. <i>Chemical Science</i> , 2022, 13, 781-788.	7.4	14
4	Remarkable CO tolerance of Ni <sup>3+</sup> active species in a Ni <sub>2</sub> O <sub>3</sub> catalyst for sustained electrochemical urea oxidation. <i>Journal of Materials Chemistry A</i> , 2022, 10, 4209-4221.	10.3	57
5	Metal-free Kinugasa reaction catalyzed by external electric field. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	1.9	8
6	A Hierarchical (Macro)molecular Assembly Assisted by Donor-Acceptor Charge-Transfer Interactions Exhibiting Room-Temperature Ferroelectricity. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	13
7	Adsorbate-Induced Phase Transformation of Ambient Stable Noncubic Lattices in Au Microcrystallites. <i>Journal of Physical Chemistry C</i> , 2022, 126, 823-831.	3.1	3
8	Deciphering the Role of Substitution in Transition-Metal Phosphorous Trisulfide (100) Surface: A Highly Efficient and Durable Pt-free ORR Electrocatalyst. <i>ChemPhysChem</i> , 2022, 23, .	2.1	1
9	Epitaxial Orientation Angle Tuned Disk-on-Rod Nanoheterostructures for Boosting Charge Transfer. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3804-3811.	4.6	2
10	Thiazole Containing PNA Mimic Regulates c-MYC Gene Expression through DNA G-Quadruplex. <i>Bioconjugate Chemistry</i> , 2022, 33, 1145-1155.	3.6	2
11	Rational Design of Biaxial Tensile Strain for Boosting Electronic and Ionic Conductivities of Na <sub>2</sub> MnSiO <sub>4</sub> for Rechargeable Sodium-Ion Batteries. <i>ChemistryOpen</i> , 2022, 11, .	1.9	3
12	Compression Produces a Square-Planar Iron Tetracarbonyl. <i>Inorganic Chemistry</i> , 2022, 61, 9055-9062.	4.0	1
13	Performance of the nitrogen reduction reaction on metal bound g-C <sub>6</sub> N <sub>6</sub> : a combined approach of machine learning and DFT. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17050-17058.	2.8	15
14	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp <sup>2</sup> )-H Activation in Conformationally Flexible Arylammonium Salts. <i>Journal of Organic Chemistry</i> , 2022, 87, 9222-9231.	3.2	2
15	Designing C <sub>6</sub> N <sub>6</sub> /C <sub>2</sub> N van der Waals heterostructures for photogenerated charge carrier separation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3925-3933.	2.8	25
16	Molecular Mechanism for the Self-Supported Synthesis of Graphitic Carbon Nitride from Urea Pyrolysis. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1396-1406.	4.6	20
17	Evolutionary structure prediction-assisted design of anode materials for Ca-ion battery based on phosphorene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9466-9475.	2.8	13
18	Prolinamide plays a key role in promoting copper-catalyzed cycloaddition of azides and alkynes in aqueous media via unprecedented metallacycle intermediates. <i>Organic Chemistry Frontiers</i> , 2021, 8, 2434-2441.	4.5	5

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19	Nickel-cobalt oxalate as an efficient non-precious electrocatalyst for an improved alkaline oxygen evolution reaction. <i>Nanoscale Advances</i> , 2021, 3, 3770-3779.	4.6	19
20	Tuning of the optoelectronic properties of peptide-appended core-substituted naphthalenediimides: the role of self-assembly of two positional isomers. <i>Soft Matter</i> , 2021, 17, 7168-7176.	2.7	9
21	Tuning intermediate adsorption in structurally ordered substituted PdCu <sub>3</sub> intermetallic nanoparticles for enhanced ethanol oxidation reaction. <i>Chemical Communications</i> , 2021, 57, 4508-4511.	4.1	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. <i>ACS Applied Energy Materials</i> , 2021, 4, 3017-3032.	5.1	9
23	Molecular Dynamics Simulations Reveal Orientation-Dependent Nanotoxicity of Black Phosphorene toward Dimeric Proteins. <i>ACS Applied Nano Materials</i> , 2021, 4, 3095-3107.	5.0	15
24	Novel Tetradentate Phosphonate Ligand Based Bioinspired Co-Metal-Organic Frameworks: Robust Electrocatalyst for the Hydrogen Evolution Reaction in Different Mediums. <i>Crystal Growth and Design</i> , 2021, 21, 2614-2623.	3.0	17
25	Formation of Metallic Polyferrocene Chains under Pressure. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3362-3368.	2.5	6
26	Synthetic and Computational Studies on Rh <sup>III</sup> -Catalyzed Redox-Neutral Cascade of Carbenoid Functionalization and Dephosphonylative Annulation. <i>Journal of Organic Chemistry</i> , 2021, 86, 7069-7077.	3.2	13
27	An NHC-Stabilised Phosphinidene for Catalytic Formylation: A DFT-Guided Approach. <i>Chemistry - A European Journal</i> , 2021, 27, 11656-11662.	3.3	6
28	Direct CO <sub>2</sub> capture and conversion to fuels on magnesium nanoparticles under ambient conditions simply using water. <i>Chemical Science</i> , 2021, 12, 5774-5786.	7.4	25
29	Harnessing Noncovalent Interactions for a Directed Evolution of a Six-Component Molecular Crystal. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12584-12591.	2.6	6
30	Gold-Catalyzed Cross-Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. <i>Chemistry - A European Journal</i> , 2020, 26, 1442-1487.	3.3	128
31	Screening two dimensional materials for the transportation and delivery of diverse genetic materials. <i>Nanoscale</i> , 2020, 12, 703-719.	5.6	23
32	Harnessing the Efficacy of 2-Pyridone Ligands for Pd-Catalyzed (I <sup>2</sup> /I <sup>3</sup> )-C(sp <sup>3</sup> )-H Activations. <i>Journal of Organic Chemistry</i> , 2020, 85, 13228-13238.	3.2	22
33	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24451-24459.	3.1	13
34	Cobalt phthalocyanine (CoPc) monolayer: A computational study on oxygen reduction reaction (ORR). <i>AIP Conference Proceedings</i> , 2020, , .	0.4	0
35	Molecular designs for expanding the limits of ultralong C-C bonds and ultrashort H-H non-bonded contacts. <i>Chemical Communications</i> , 2020, 56, 15377-15386.	4.1	12
36	Heavy-atom tunneling in organic transformations. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	1.5	8

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37	Deoxygenation of nitrosoarene by N-heterocyclic carbene (NHC): an elusive Breslow-type intermediate bridging carbene and nitrene. <i>Chemical Communications</i> , 2020, 56, 12166-12169.	4.1	2
38	Paradoxical design of a serendipitous pyrazolate bridging mode: a pragmatic strategy for inducing ineluctable ferromagnetic coupling. <i>Dalton Transactions</i> , 2020, 49, 13704-13716.	3.3	2
39	Disentangling the liquid phase exfoliation of two-dimensional materials: an <i>in silico</i> perspective. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22157-22179.	2.8	17
40	Polymorphism Dependent 9-Phosphoanthracene Derivative Exhibiting Thermally Activated Delayed Fluorescence: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 11025-11037.	2.5	17
41	Enhanced Photophysical Properties of Bi <sub>2</sub> S <sub>3</sub> /AgBiS <sub>2</sub> Nanoheterostructures Synthesized via Ag(I) Cation Exchange-Mediated Transformation of Binary Bi <sub>2</sub> S <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2020, 124, 12824-12833.	3.1	5
42	Transition-Metal Phosphorus Trisulfides and its Vacancy Defects: Emergence of a New Class of Anode Material for Li-Ion Batteries. <i>ChemSusChem</i> , 2020, 13, 3855-3864.	6.8	30
43	Delicate Balance of Non-Covalent Forces Govern the Biocompatibility of Graphitic Carbon Nitride towards Genetic Materials. <i>ChemPhysChem</i> , 2020, 21, 1836-1846.	2.1	12
44	Defects in nanosilica catalytically convert CO <sub>2</sub> to methane without any metal and ligand. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 6383-6390.	7.1	68
45	Frontispiece: Gold-Catalyzed Cross-Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. <i>Chemistry - A European Journal</i> , 2020, 26, .	3.3	1
46	Transition-State-like Planar Structures for Amine Inversion with Ultralong C-C Bonds in Diamino-carborane and Diamino-dodecahedron. <i>Journal of the American Chemical Society</i> , 2020, 142, 5331-5337.	13.7	18
47	Enhancement in electrical conductivity of a porous indium based metal-organic framework upon I <sub>2</sub> uptake: combined experimental and theoretical investigations. <i>Journal of Materials Chemistry C</i> , 2020, 8, 4836-4842.	5.5	13
48	A Thiadiazole-Based Covalent Organic Framework: A Metal-Free Electrocatalyst toward Oxygen Evolution Reaction. <i>ACS Catalysis</i> , 2020, 10, 5623-5630.	11.2	140
49	Remote Functionalization through Symmetric or Asymmetric Substitutions Control the Pathway of Intermolecular Singlet Fission. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5014-5023.	5.3	9
50	Hierarchical Noncovalent Interactions between Molecules Stabilize Multicomponent Cocrystals. <i>Crystal Growth and Design</i> , 2019, 19, 4802-4809.	3.0	14
51	Pt/Co <sub>3</sub> O <sub>4</sub> Surpasses Benchmark Pt/C: An Approach Toward Next Generation Hydrogen Evolution Electrocatalyst. <i>ACS Applied Energy Materials</i> , 2019, 2, 5613-5621.	5.1	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. <i>New Journal of Chemistry</i> , 2019, 43, 15311-15315.	2.8	3
53	Influence of Axial Linkers on Polymerization in Paddle-Wheel Cu(II) Coordination Polymers for the Application of Optoelectronics Devices. <i>Crystal Growth and Design</i> , 2019, 19, 6283-6290.	3.0	20
54	Transforming atmospheric CO <sub>2</sub> into alternative fuels: a metal-free approach under ambient conditions. <i>Chemical Science</i> , 2019, 10, 1879-1884.	7.4	19

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55	Aryl-platform-based tetrapodal 2-iodo-imidazolium as an excellent halogen bond receptor in aqueous medium. <i>Chemical Communications</i> , 2019, 55, 1506-1509.	4.1	22
56	Topological Phase Transition in $Sb_2Mg_3$ Assisted by Strain. <i>ACS Omega</i> , 2019, 4, 8701-8706.	3.5	11
57	Visible light driven efficient metal free single atom catalyst supported on nanoporous carbon nitride for nitrogen fixation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12346-12352.	2.8	64
58	Computationally Driven Design Principles for Singlet Fission in Organic Chromophores. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19257-19268.	3.1	22
59	A Solution Processed Ultrathin Molecular Dielectric for Organic Field-Effect Transistors. <i>ACS Applied Electronic Materials</i> , 2019, 1, 485-493.	4.3	4
60	Analysis of pseudo jahn-teller distortion based on natural bond orbital theory: Case study for silicene. <i>Journal of Computational Chemistry</i> , 2019, 40, 1488-1495.	3.3	14
61	Aggregation induced non-emissive-to-emissive switching of molecular platinum clusters. <i>Nanoscale</i> , 2019, 11, 5914-5919.	5.6	13
62	Intramolecular Singlet Fission in Quinoidal Dihydrothiophene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4749-4754.	3.1	10
63	Interaction of a bioactive molecule with surfaces of nanoscale transition metal oxides: experimental and theoretical studies. <i>New Journal of Chemistry</i> , 2019, 43, 16621-16628.	2.8	4
64	Red-Emitting Copper Nanoclusters: From Bulk-Scale Synthesis to Catalytic Reduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 1998-2007.	6.7	46
65	Gauging the Nanotoxicity of $h_2D-C_2N$ toward Single-Stranded DNA: An in Silico Molecular Simulation Approach. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 13805-13818.	8.0	39
66	Controlled Pore Sizes in Monolayer $C_2N$ Act as Ultrasensitive Probes for Detection of Gaseous Pollutants (HF, HCN, and $H_2S$ ). <i>Journal of Physical Chemistry C</i> , 2018, 122, 2248-2258.	3.1	53
67	Dynamical Effects along the Bifurcation Pathway Control Semibullvalene Formation in Deazetization Reactions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1239-1244.	2.6	14
68	Topological Insulator in Two-Dimensional SiGe Induced by Biaxial Tensile Strain. <i>ACS Omega</i> , 2018, 3, 1-7.	3.5	23
69	Novel Br $\pi$ -(Chelate) Interaction in a 1D Coordination Polymer Revealing Aromaticity. <i>ChemistrySelect</i> , 2018, 3, 4289-4291.	1.5	18
70	Evidence of homo-FRET in quantum dot dye heterostructured assembly. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9523-9535.	2.8	23
71	Ultrafast Relaxation Dynamics of Luminescent Copper Nanoclusters ( $Cu_7L_3$ ) and Efficient Electron Transfer to Functionalized Reduced Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13354-13362.	3.1	44
72	Structure and Electronic Properties of Unnatural Base Pairs: The Role of Dispersion Interactions. <i>ChemPhysChem</i> , 2018, 19, 67-74.	2.1	16

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73	A Vision on Organosilicon Chemistry and Silicene. <i>Nanoscience and Technology</i> , 2018, , 1-21.	1.5	2
74	Silicon-Doped Nitrogen-Coordinated Graphene as Electrocatalyst for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27233-27240.	3.1	59
75	Design Rules for the Generation of Stable Quartet Phases of Nucleobases over Two-Dimensional Materials. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28918-28933.	3.1	26
76	Strain-Induced Topological Insulator in Methyl-Decorated SiGe Films. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25127-25133.	3.1	12
77	Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. <i>Inorganic Chemistry</i> , 2018, 57, 11995-12009.	4.0	29
78	Doped boron nitride surfaces: potential metal free bifunctional catalysts for non-aqueous Li <sup>+</sup> O <sub>2</sub> batteries. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16485-16492.	2.8	10
79	Reactive Molecular Dynamics Simulations of Self-Assembly of Polytwistane and Its Application for Nanofibers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19204-19211.	3.1	11
80	Gold(I)-Catalyzed Intramolecular Diels-Alder Reaction: Evolution of Trappable Intermediates via Asynchronous Transition States. <i>Journal of Organic Chemistry</i> , 2018, 83, 11167-11177.	3.2	19
81	Understanding Thermal and Photochemical Aryl-Aryl Cross-Coupling by the Au <sup>I</sup> /Au <sup>III</sup> Redox Couple. <i>Chemistry - A European Journal</i> , 2018, 24, 13636-13646.	3.3	21
82	Pseudo-Jahn-Teller effects in two-dimensional silicene, germanene and stanene: a crystal orbital vibronic coupling density analysis. <i>Bulletin of Materials Science</i> , 2018, 41, 1.	1.7	5
83	An Azoaromatic Ligand as Four Electron Four Proton Reservoir: Catalytic Dehydrogenation of Alcohols by Its Zinc(II) Complex. <i>Inorganic Chemistry</i> , 2018, 57, 6816-6824.	4.0	45
84	Noble-Metal-Supported GeS Monolayer as Promising Single-Atom Catalyst for CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14488-14498.	3.1	35
85	Phase Coexistence and Strain-Induced Topological Insulator in Two-Dimensional BiAs. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15047-15054.	3.1	33
86	Tunneling Control: Competition between 6 $\pi$ -Electrocyclization and [1,5]H-Sigmatropic Shift Reactions in Tetrahydro-1 <i>H</i> -cyclobuta[ <i>e</i> ]indene Derivatives. <i>Journal of Organic Chemistry</i> , 2017, 82, 1558-1566.	3.2	23
87	Direct and Autocatalytic Reductive Elimination from Gold Complexes ((Ph) <sub>3</sub> P)Au(Ar)(CF <sub>3</sub> ) <sub>3</sub> (X)], X=F, Cl, Br, I): The Key Role of Halide Ligands. <i>Chemistry - A European Journal</i> , 2017, 23, 4169-4179.	3.3	31
88	Polymorphism Controlled Singlet Fission in TIPS-Anthracene: Role of Stacking Orientation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1412-1420.	3.1	60
89	Size specific emission in peptide capped gold quantum clusters with tunable photoswitching behavior. <i>Nanoscale</i> , 2017, 9, 4419-4429.	5.6	32
90	Ordering and Dynamics for the Formation of Two-Dimensional Molecular Crystals on Black Phosphorene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 10210-10223.	3.1	43

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91	Exotic Physics and Chemistry of Two-Dimensional Phosphorus: Phosphorene. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2909-2916.	4.6	71
92	Theoretical study of Au 4 thymine, Au 20 and Ag 20 uracil and thymine complexes for surface enhanced Raman scattering. <i>Computational and Theoretical Chemistry</i> , 2017, 1111, 1-13.	2.5	15
93	Monolayer Group IV-VI Monochalcogenides: Low-Dimensional Materials for Photocatalytic Water Splitting. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7615-7624.	3.1	154
94	Design of van der Waals Two-Dimensional Heterostructures from Facially Polarized Janus All-Cis 1,2,3,4,5,6-Hexafluorocyclohexane (C6H6F6). <i>Journal of Physical Chemistry C</i> , 2017, 121, 1752-1762.	3.1	18
95	Exploring Ultrashort Hydrogen-Hydrogen Nonbonded Contacts in Constrained Molecular Cavities. <i>Journal of Physical Chemistry B</i> , 2017, 121, 825-834.	2.6	23
96	Deciphering the Role of Solvents in the Liquid Phase Exfoliation of Hexagonal Boron Nitride: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 811-822.	3.1	59
97	Influence of Hofmeister I <sup>+</sup> on Tuning Optoelectronic Properties of Ampholytic Polythiophene by Varying pH and Conjugating with RNA. <i>Langmuir</i> , 2017, 33, 12739-12749.	3.5	16
98	Role of Carbon Support for Subnanometer Gold-Cluster-Catalyzed Disiloxane Synthesis from Hydrosilane and Water. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20101-20112.	3.1	9
99	Two-Dimensional Graphene-Gold Interfaces Serve as Robust Templates for Dielectric Capacitors. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 34213-34220.	8.0	28
100	Visible-Light-Mediated Excited State Relaxation in Semi-Synthetic Genetic Alphabet: d5SICS and dNaM. <i>Chemistry - A European Journal</i> , 2017, 23, 11494-11498.	3.3	16
101	Understanding the Reactivity of CO <sub>3</sub> <sup>•-</sup> and NO <sub>2</sub> <sup>•</sup> Radicals toward S-Containing and Aromatic Amino Acids. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7621-7632.	2.6	10
102	Coexistence of Normal and Auxetic Behavior in a Thermally and Chemically Stable sp <sup>3</sup> Nanowire: Poly[5]asterane. <i>Chemistry - A European Journal</i> , 2017, 23, 12917-12923.	3.3	12
103	External electric field control: driving the reactivity of metal-free azide-alkyne click reactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22482-22486.	2.8	47
104	Effect of Doping in Controlling the Structure, Reactivity, and Electronic Properties of Pristine and Ca(II)-Intercalated Layered Silicene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15169-15180.	3.1	17
105	Janus all-cis-1,2,3,4,5,6-Hexafluorocyclohexane: A Molecular Motif for Aggregation-Induced Enhanced Polarization. <i>ChemPhysChem</i> , 2016, 17, 2373-2381.	2.1	29
106	Classroom. <i>Resonance</i> , 2016, 21, 377-379.	0.3	0
107	Controlling electronic effects and intermolecular packing in contorted polyaromatic hydrocarbons (c-PAHs): towards high mobility field effect transistors. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14886-14893.	2.8	11
108	Supported Sub-Nanometer Gold Cluster Catalyzed Transfer Hydrogenation of Aldehydes to Alcohols. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24449-24456.	3.1	14

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109	Exclusively Ligand-Mediated Catalytic Dehydrogenation of Alcohols. <i>Inorganic Chemistry</i> , 2016, 55, 9602-9610.	4.0	55
110	Nonequimolar Mixture of Organic Acids and Bases: An Exception to the Rule of Thumb for Salt or Cocrystal. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7606-7613.	2.6	25
111	Metal-Free Reduction of CO <sub>2</sub> to Methoxyborane under Ambient Conditions through Borondiformate Formation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15147-15151.	13.8	50
112	Steric and electric field driven distortions in aromatic molecules: spontaneous and non-spontaneous symmetry breaking. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31160-31167.	2.8	23
113	Two-Dimensional Group IV Monochalcogenides: Anode Materials for Li-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14522-14530.	3.1	120
114	Capping Black Phosphorene by h-BN Enhances Performances in Anodes for Li and Na Ion Batteries. <i>ACS Energy Letters</i> , 2016, 1, 253-259.	17.4	126
115	Multifunctional mixed ligand metal organic frameworks: X-ray structure, adsorption, luminescence and electrical conductivity with theoretical correlation. <i>CrystEngComm</i> , 2016, 18, 5754-5763.	2.6	23
116	Role of Heavy Atom Tunneling in Myers-Saito Cyclization of Cyclic Enyne-Cumulene Systems. <i>Journal of Physical Chemistry B</i> , 2016, 120, 945-950.	2.6	26
117	Dual Fluorescence in GFP Chromophore Analogues: Chemical Modulation of Charge Transfer and Proton Transfer Bands. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3503-3510.	2.6	26
118	Pseudo-Jahn-Teller Distortion in Two-Dimensional Phosphorus: Origin of Black and Blue Phases of Phosphorene and Band Gap Modulation by Molecular Charge Transfer. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1288-1297.	4.6	73
119	Strain Control: Reversible H <sub>2</sub> Activation and H <sub>2</sub> /D <sub>2</sub> Exchange in Pt Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 3023-3029.	4.0	18
120	Pseudo Jahn-Teller distortion for a tricyclic carbon sulfide (C <sub>6</sub> S <sub>8</sub> ) and its suppression in S-oxygenated dithiine (C <sub>4</sub> H <sub>4</sub> (SO <sub>2</sub> ) <sub>2</sub> ). <i>Chemical Physics</i> , 2015, 460, 101-105.	1.9	27
121	Topochemical Transformations of CaX <sub>2</sub> (X=C, Si, Ge) to Form Free-Standing Two-Dimensional Materials. <i>Chemistry - A European Journal</i> , 2015, 21, 18454-18460.	3.3	31
122	Fluorescence from an H-aggregated naphthalenediimide based peptide: photophysical and computational investigation of this rare phenomenon. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30398-30403.	2.8	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. <i>Journal of Physical Chemistry C</i> , 2015, 119, 926-933.	3.1	14
124	Electronic and Chemical Properties of Germanene: The Crucial Role of Buckling. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3802-3809.	3.1	125
125	1,4-Dithiine Puckered in the Gas Phase but Planar in Crystals: Role of Cooperativity. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15770-15776.	3.1	22
126	Half-sandwich Ru( <sup>η</sup> -C <sub>6</sub> H <sub>6</sub> ) complexes with chiral aroylthioureas for enhanced asymmetric transfer hydrogenation of ketones – experimental and theoretical studies. <i>Catalysis Science and Technology</i> , 2015, 5, 4790-4799.	4.1	28



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127	What Sustains the Unnatural Base Pairs (UBPs) with No Hydrogen Bonds. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5839-5845.	2.6	36
128	Mechanistic insights into the synergistic catalysis by Au(I), Ga(III), and counterions in the Nakamura reaction. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 7412-7420.	2.8	28
129	Small Organic Molecules for Efficient Singlet Fission: Role of Silicon Substitution. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25696-25702.	3.1	36
130	Metal Free Azide-Alkyne Click Reaction: Role of Substituents and Heavy Atom Tunneling. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11540-11547.	2.6	23
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