Ayan Datta

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/824431/publications.pdf

Version: 2024-02-01

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	Structures and Chemical Properties of Silicene: Unlike Graphene. Accounts of Chemical Research, 2014, 47, 593-602.	7.6	291
2	Dipolar interactions and hydrogen bonding in supramolecular aggregates: understanding cooperative phenomena for 1st hyperpolarizability. Chemical Society Reviews, 2006, 35, 1305.	18.7	227
3	Understanding of the Buckling Distortions in Silicene. Journal of Physical Chemistry C, 2012, 116, 24639-24648.	1.5	188
4	Monolayer Group IVâ€“VI Monochalcogenides: Low-Dimensional Materials for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2017, 121, 7615-7624.	1.5	154
5	A Thiadiazole-Based Covalent Organic Framework: A Metal-Free Electrocatalyst toward Oxygen Evolution Reaction. ACS Catalysis, 2020, 10, 5623-5630.	5.5	140
6	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
7	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
8	Structures and electronic properties of silicene clusters: a promising material for FET and hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 7304.	1.3	125
9	Electronic and Chemical Properties of Germanene: The Crucial Role of Buckling. Journal of Physical Chemistry C, 2015, 119, 3802-3809.	1.5	125
10	Two-Dimensional Group IV Monochalcogenides: Anode Materials for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 14522-14530.	1.5	120
11	Dipole orientation effects on nonlinear optical properties of organic molecular aggregates. Journal of Chemical Physics, 2003, 118, 8420-8427.	1.2	117
12	Experimental Evidence for Heavy-Atom Tunneling in the Ring-Opening of Cyclopropylcarbinyl Radical from Intramolecular ¹²C/¹³C Kinetic Isotope Effects. Journal of the American Chemical Society, 2010, 132, 12548-12549.	6.6	84
13	Nitroxyl Radical Plus Hydroxylamine Pseudo Self-Exchange Reactions: Tunneling in Hydrogen Atom Transfer. Journal of the American Chemical Society, 2009, 131, 11985-11997.	6.6	81
14	Electron and hole mobilities in polymorphs of benzene and naphthalene: Role of intermolecular interactions. Journal of Chemical Physics, 2007, 126, 144710.	1.2	78
15	Molecular Balances Based on Aliphatic CHâ‹¯Ï€ and Lone-Pairâ‹¯Ï€ Interactions. Journal of Physical Chemistry Letters, 2012, 3, 1493-1496.	2.1	78
16	Highâ€Mobility Field Effect Transistors Based on Supramolecular Charge Transfer Nanofibres. Advanced Materials, 2013, 25, 559-564.	11.1	74
17	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
18	Exotic Physics and Chemistry of Two-Dimensional Phosphorus: Phosphorene. Journal of Physical Chemistry Letters, 2017, 8, 2909-2916.	2.1	71

#	Article	IF	Citations
19	Charge-Transfer Induced Large Nonlinear Optical Properties of Small Al Clusters:â€‰ Al4M4 (M = Li, Na,) Tj ETQq1 1 0.784314 rgBT /	1.1	68
20	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
21	Comparing the electron and hole mobilities in the Î± and Î² phases of perylene: role of Ï€-stacking. Journal of Materials Chemistry, 2007, 17, 1933-1938.	6.7	67
22	Competing Magnetic Interactions in a Dinuclear Ni(II) Complex:Â Antiferromagnetic Oâˆ'HÂ·Â·Â·O Moiety and Ferromagnetic N3-Ligand. Journal of Physical Chemistry B, 2006, 110, 12-15.	1.2	66
23	Nucleic Acid G-quartets: Insights into Diverse Patterns and Optical Properties. Journal of Physical Chemistry C, 2011, 115, 12530-12546.	1.5	64
24	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
25	Polymorphism Controlled Singlet Fission in TIPS-Anthracene: Role of Stacking Orientation. Journal of Physical Chemistry C, 2017, 121, 1412-1420.	1.5	60
26	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
27	Silicon-Doped Nitrogen-Coordinated Graphene as Electrocatalyst for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 27233-27240.	1.5	59
28	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
29	Stable Transition Metal Complexes of an All-Metal Antiaromatic Molecule (Al4Li4):Â Role of Complexations. Journal of the American Chemical Society, 2005, 127, 3496-3500.	6.6	56
30	Calculations Predict Rapid Tunneling by Carbon from the Vibrational Ground State in the Ring Opening of Cyclopropylcarbinyl Radical at Cryogenic Temperatures. Journal of the American Chemical Society, 2008, 130, 6684-6685.	6.6	56
31	Exclusively Ligand-Mediated Catalytic Dehydrogenation of Alcohols. Inorganic Chemistry, 2016, 55, 9602-9610.	1.9	55
32	Quantifying Aromaticity at the Molecular and Supramolecular Limits:â€‰ Comparing Homonuclear, Heteronuclear, and H-Bonded Systems. Journal of Chemical Theory and Computation, 2006, 2, 30-36.	2.3	54
33	Designing Molecular Switches Based on DNA-Base Mispairing. Journal of Physical Chemistry B, 2010, 114, 15311-15318.	1.2	54
34	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
35	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
36	Metalâ€Free Reduction of CO₂ to Methoxyborane under Ambient Conditions through Borondiformate Formation. Angewandte Chemie - International Edition, 2016, 55, 15147-15151.	7.2	50

#	Article	IF	Citations
37	Nonlocal Electronic Distribution in Metallic Clusters:â€‰ A Critical Examination of Aromatic Stabilization. Accounts of Chemical Research, 2007, 40, 213-221.	7.6	49
38	Nanoparticle-Catalyzed Clock Reaction. Journal of Physical Chemistry C, 2008, 112, 3619-3626.	1.5	49
39	Effect of External Electric Field on Hâ€Bonding and Ïâ€Stacking Interactions in Guanine Aggregates. ChemPhysChem, 2012, 13, 4163-4172.	1.0	48
40	A charge transfer single crystal field effect transistor operating at low voltages. Chemical Communications, 2013, 49, 5847.	2.2	48
41	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
42	Computational Design of High Hydrogen Adsorption Efficiency in Molecular â€œSulflowerâ€• Journal of Physical Chemistry C, 2007, 111, 4487-4490.	1.5	47
43	Role of Metal Ions (M = Li⁺, Na⁺, and K⁺) and Pore Sizes (Crown-4,) Tj ETQq1 1 0.784314 rgBT /O Birefringence. Journal of Physical Chemistry C, 2009, 113, 3339-3344.	1.5	47
44	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
45	Modulation of Fluorescence Resonance Energy Transfer Efficiency for White Light Emission from a Series of Stilbene-Perylene Based Donorâ€“Acceptor Pair. Journal of Physical Chemistry C, 2013, 117, 23178-23189.	1.5	46
46	Red-Emitting Copper Nanoclusters: From Bulk-Scale Synthesis to Catalytic Reduction. ACS Sustainable Chemistry and Engineering, 2019, 7, 1998-2007.	3.2	46
47	Role of Nonbonding Interactions in the Crystal Growth of Phenazinediamine Tetrahydrate:â€‰ New Insights into the Occurrence of 2D Water Layers in Crystal Hydrates. Crystal Growth and Design, 2007, 7, 966-971.	1.4	45
48	Role of Multicentered Bonding in Controlling Magnetic Interactions in Ï€-Stacked Bis-dithiazolyl Radical. Crystal Growth and Design, 2011, 11, 3137-3140.	1.4	45
49	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
50	Computational design of concomitant type-I and type-II porphyrin sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 18471.	1.3	44
51	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
52	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
53	Effects of Dipole Orientations on Nonlinear Optical Properties of Oxo-Bridged Dinitroaniline Systems. Journal of Physical Chemistry A, 2004, 108, 320-325.	1.1	43
54	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

#	Article	IF	Citations
55	Design and Applications of Noncanonical DNA Base Pairs. Journal of Physical Chemistry Letters, 2014, 5, 154-166.	2.1	41
56	Phenalenyl in a Different Role: Catalytic Activation through the Nonbonding Molecular Orbital. ACS Catalysis, 2014, 4, 4307-4319.	5.5	40
57	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
58	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
59	Do Cationâ‹…â‹…â‹…Ï€ Interactions Always Need to be 1:1?. ChemPhysChem, 2012, 13, 695-698.	1.0	37
60	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.	1.2	36
61	Synthesis, Structure, and Transformation Studies in a Family of Inorganicâ"Organic Hybrid Framework Structures Based on Indium. Inorganic Chemistry, 2009, 48, 11697-11711.	1.9	36
62	Oddâ€"even oscillations in structural and optical properties of gold clusters. Computational and Theoretical Chemistry, 2010, 945, 93-96.	1.5	36
63	Tunneling Assists the 1,2â€Hydrogen Shift in Nâ€Heterocyclic Carbenes. Angewandte Chemie - International Edition, 2014, 53, 9587-9591.	7.2	36
64	What Sustains the Unnatural Base Pairs (UBPs) with No Hydrogen Bonds. Journal of Physical Chemistry B, 2015, 119, 5839-5845.	1.2	36
65	Small Organic Molecules for Efficient Singlet Fission: Role of Silicon Substitution. Journal of Physical Chemistry C, 2015, 119, 25696-25702.	1.5	36
66	Nonlinear Optical Properties in Calix[n]arenes: Orientation Effects of Monomers. Chemistry - A European Journal, 2005, 11, 4961-4969.	1.7	35
67	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
68	Structures and Electronic Properties of Si-Substituted Benzenes and Their Transition-Metal Complexes. Journal of Physical Chemistry Letters, 2010, 1, 136-140.	2.1	34
69	Cooperative Interactions in Supramolecular Aggregates: Linear and Nonlinear Responses in Calix[4]arenes. ChemPhysChem, 2006, 7, 2168-2174.	1.0	33
70	Mechanistic Study for the Facile Oxidation of Trimethoprim on a Manganese Porphyrin Incorporated Glassy Carbon Electrode. Journal of Physical Chemistry C, 2011, 115, 21858-21864.	1.5	33
71	Why Does Gold(III) Porphyrin Act as a Selective Catalyst in the Cycloisomerization of Allenones?. Journal of Physical Chemistry C, 2011, 115, 2187-2195.	1.5	33
72	Phase Coexistence and Strain-Induced Topological Insulator in Two-Dimensional BiAs. Journal of Physical Chemistry C, 2018, 122, 15047-15054.	1.5	33

#	Article	IF	Citations
73	Aromaticity in Stable Tiara Nickel Thiolates:â€‰ Computational and Structural Analysis. Journal of Physical Chemistry A, 2005, 109, 11647-11649.	1.1	32
74	Calculations Predict a Large Inverse H/D Kinetic Isotope Effect on the Rate of Tunneling in the Ring Opening of Cyclopropylcarbinyl Radical. Journal of the American Chemical Society, 2009, 131, 16002-16003.	6.6	32
75	Size specific emission in peptide capped gold quantum clusters with tunable photoswitching behavior. Nanoscale, 2017, 9, 4419-4429.	2.8	32
76	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
77	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
78	Magnetic Interactions in Layered Nickel Alkanethiolates. Journal of Physical Chemistry C, 2007, 111, 1868-1870.	1.5	30
79	What Stabilizes the Li_nP_n Inorganic Double Helices?. Journal of Physical Chemistry Letters, 2013, 4, 1018-1022.	2.1	30
80	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
81	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
82	Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. Inorganic Chemistry, 2018, 57, 11995-12009.	1.9	29
83	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
84	Calculations Find That Tunneling Plays a Major Role in the Reductive Elimination of Methane from Hydridomethylbis(trimethylphosphine)platinum:â€‰ How to Confirm This Computational Prediction Experimentally. Journal of the American Chemical Society, 2008, 130, 2726-2727.	6.6	28
85	Mechanism for Câ€“I Bond Dissociation in Iodoethane, Iodobenzene, and Iodoethene for the Câ€“C Cross Coupling Reactions over Gold Clusters. Journal of Physical Chemistry C, 2013, 117, 21433-21440.	1.5	28
86	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
87	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
88	Two-Dimensional Grapheneâ€“Gold Interfaces Serve as Robust Templates for Dielectric Capacitors. ACS Applied Materials & Interfaces, 2017, 9, 34213-34220.	4.0	28
89	Effects of conjugation length and donorâ€“acceptor functionalization on the non-linear optical properties of organic pushâ€“pull molecules using density functional theory. Computational and Theoretical Chemistry, 2005, 715, 59-64.	1.5	27
90	Can Arsenates Replace Phosphates in Natural Biochemical Processes? A Computational Study. Journal of Physical Chemistry B, 2013, 117, 8340-8346.	1.2	27

#	Article	IF	Citations
91	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
92	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
93	Tip enhanced Raman spectroscopy (TERS) as a probe for the buckling distortion in silicene. Physical Chemistry Chemical Physics, 2013, 15, 8700.	1.3	26
94	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
95	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
96	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
97	Rationalization of the Ï€â^Ïƒ (Anti)aromaticity in All Metal Molecular Clusters. Journal of Chemical Theory and Computation, 2005, 1, 824-826.	2.3	25
98	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
99	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
100	Designing C₆N₆/C₂N van der Waals heterostructures for photogenerated charge carrier separation. Physical Chemistry Chemical Physics, 2021, 23, 3925-3933.	1.3	25
101	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
102	New examples of metalloaromatic Al-clusters: (Al4M4)Fe(CO)3(M = Li, Na and K) and (Al4M4)2Ni: rationalization for possible synthesis. Chemical Communications, 2005, , 5032.	2.2	23
103	Structure and electronic properties of the Watsonâ€“Crick base pairs: Role of hydrogen bonding. Synthetic Metals, 2005, 155, 398-401.	2.1	23
104	Aromatic Superclusters from All-Metal Aromatic and Antiaromatic Monomers, [Al4]2-and [Al4]4-. Journal of Physical Chemistry B, 2006, 110, 20098-20101.	1.2	23
105	Tunneling Governs Intramolecular Proton Transfer in Thiotropolone at Room Temperature. Angewandte Chemie - International Edition, 2012, 51, 9389-9392.	7.2	23
106	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
107	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
108	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

#	Article	IF	Citations
109	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
110	Exploring Ultrashort Hydrogenâ€“Hydrogen Nonbonded Contacts in Constrained Molecular Cavities. Journal of Physical Chemistry B, 2017, 121, 825-834.	1.2	23
111	Topological Insulator in Two-Dimensional SiGe Induced by Biaxial Tensile Strain. ACS Omega, 2018, 3, 1-7.	1.6	23
112	Evidence of homo-FRET in quantum dotâ€“dye heterostructured assembly. Physical Chemistry Chemical Physics, 2018, 20, 9523-9535.	1.3	23
113	Screening two dimensional materials for the transportation and delivery of diverse genetic materials. Nanoscale, 2020, 12, 703-719.	2.8	23
114	How Stable are the Mgâˆ’Mg Bonds in Magnesium (I) Compounds toward Hydrogenation?. Journal of Physical Chemistry C, 2008, 112, 18727-18729.	1.5	22
115	Molecular Rotor Inside a Phosphonate Cavitand: Role of Supramolecular Interactions. Journal of Physical Chemistry Letters, 2010, 1, 1363-1366.	2.1	22
116	Metal encapsulation mediated planar to three dimensional structural transformation in Au-clusters: The venus flytrap effect. Computational and Theoretical Chemistry, 2011, 966, 133-136.	1.1	22
117	Aminoindolines versus Quinolines: Mechanistic Insights into the Reaction between 2-Aminobenzaldehydes and Terminal Alkynes in the Presence of Metals and Secondary Amines. Journal of Organic Chemistry, 2012, 77, 6179-6185.	1.7	22
118	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
119	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
120	Computationally Driven Design Principles for Singlet Fission in Organic Chromophores. Journal of Physical Chemistry C, 2019, 123, 19257-19268.	1.5	22
121	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
122	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
123	Oddâˆ’Even Oscillations in First Hyperpolarizability of Dipolar Chromophores:Â Role of Conformations of Spacers. Journal of Physical Chemistry A, 2005, 109, 4112-4117.	1.1	20
124	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
125	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
126	Linear and nonlinear optical polarizabilities in supramolecular aggregates: Effects of hydrogen bonding and dipolar interactions. Computational and Theoretical Chemistry, 2005, 756, 97-102.	1.5	19

#	Article	IF	Citations
127	Charge density analysis of two proton transfer complexes: Understanding hydrogen bonding and determination of in-crystal dipole moments. Journal of Chemical Sciences, 2008, 120, 613-620.	0.7	19
128	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
129	Transforming atmospheric CO₂ into alternative fuels: a metal-free approach under ambient conditions. Chemical Science, 2019, 10, 1879-1884.	3.7	19
130	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
131	Hierarchical Structures in Tin(II) Oxalates. European Journal of Inorganic Chemistry, 2008, 2008, 1376-1385.	1.0	18
132	Strain Control: Reversible H₂ Activation and H₂/D₂ Exchange in Pt Complexes. Inorganic Chemistry, 2016, 55, 3023-3029.	1.9	18
133	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
134	Novel Brâ‹…â‹…â‹…Ï€(Chelate) Interaction in a 1D Coordination Polymer Revealing Aromaticity. ChemistrySelect, 2018, 3, 4289-4291.	0.7	18
135	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
136	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
137	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
138	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
139	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
140	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
141	Long-range electron transfer across aÏ€-conjugated chain: Role of electron correlations. Physical Review B, 2005, 72, .	1.1	16
142	Aqueous fluoride ion sensing by a new perylenediimide derivative: Interaction between the hydrated fluoride and the aromatic molecule. Chemical Physics Letters, 2013, 588, 76-81.	1.2	16
143	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
144	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

#	Article	IF	Citations
145	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
146	Structure and Electronic Properties of Unnatural Base Pairs: The Role of Dispersion Interactions. ChemPhysChem, 2018, 19, 67-74.	1.0	16
147	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
148	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
149	Molecular Dynamics Simulations Reveal Orientation-Dependent Nanotoxicity of Black Phosphorene toward Dimeric Proteins. ACS Applied Nano Materials, 2021, 4, 3095-3107.	2.4	15
150	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
151	Modelling doped (Ni, Pd, Pt) sulfurâ€“nitrolic systems as new motifs for storage of hydrogen. Physical Chemistry Chemical Physics, 2009, 11, 11054.	1.3	14
152	Cu/AlO(OH)-catalyzed formation of Î²-enamino ketones/esters under solvent, ligand and base free conditions â€“ experimental and computational studies. Catalysis Science and Technology, 2012, 2, 1872.	2.1	14
153	Pattern Formation Due to Fluorination on Graphene Fragments: Structures, Hopping Behavior, and Magnetic Properties. Journal of Physical Chemistry A, 2013, 117, 8506-8511.	1.1	14
154	An Interplay of Cooperativity between Cationâ‹…â‹…â‹…Ï€, Anionâ‹…â‹…â‹…Ï€ and Cï£¿Hâ‹…â‹…â‹…Anion Interactions. ChemPhysChem 2013, 14, 1149-1154.	1.0	14
155	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
156	Supported Sub-Nanometer Gold Cluster Catalyzed Transfer Hydrogenation of Aldehydes to Alcohols. Journal of Physical Chemistry C, 2016, 120, 24449-24456.	1.5	14
157	Dynamical Effects along the Bifurcation Pathway Control Semibullvalene Formation in Deazetization Reactions. Journal of Physical Chemistry B, 2018, 122, 1239-1244.	1.2	14
158	Hierarchical Noncovalent Interactions between Molecules Stabilize Multicomponent Cocrystals. Crystal Growth and Design, 2019, 19, 4802-4809.	1.4	14
159	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
160	Stable room temperature ferroelectricity in hydrogen-bonded supramolecular assemblies of ambipolar Ï€-systems. Chemical Science, 2022, 13, 781-788.	3.7	14
161	Degenerate Intermolecular and Intramolecular Proton-Transfer Reactions: Electronic Structure of the Transition States. Journal of Physical Chemistry A, 2009, 113, 8147-8151.	1.1	13
162	Cycloaddition profile of pentafulvenes with 3-oxidopyrylium betaine: experimental and theoretical investigations. Tetrahedron, 2013, 69, 9751-9760.	1.0	13

#	Article	IF	Citations
163	Reactivity of germanones: far removed from ketones â€“ a computational study. RSC Advances, 2013, 3, 24321.	1.7	13
164	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
165	Aggregation induced non-emissive-to-emissive switching of molecular platinum clusters. Nanoscale, 2019, 11, 5914-5919.	2.8	13
166	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
167	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
168	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
169	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
170	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
171	Conformational Preference in Heteroatomic Analogues of Ethane, H3Xâ‹¯YH3(X = B, Al; Y = N, P):Â Implications of Charge Transfer. Journal of Physical Chemistry A, 2006, 110, 5156-5163.	1.1	12
172	Effects of geminal methyl groups on the tunnelling rates in the ring opening of cyclopropylcarbinyl radical at cryogenic temperature. Organic and Biomolecular Chemistry, 2011, 9, 3142.	1.5	12
173	Molecular Switching Behavior in Isosteric DNA Base Pairs. ChemPhysChem, 2013, 14, 1219-1226.	1.0	12
174	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
175	Strain-Induced Topological Insulator in Methyl-Decorated SiGe Films. Journal of Physical Chemistry C, 2018, 122, 25127-25133.	1.5	12
176	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
177	Delicate Balance of Nonâ€Covalent Forces Govern the Biocompatibility of Graphitic Carbon Nitride towards Genetic Materials. ChemPhysChem, 2020, 21, 1836-1846.	1.0	12
178	Limit to puckering of benzene with sterically crowded molecules: Hexaferrocenylbenzene. Chemical Physics Letters, 2006, 433, 67-70.	1.2	11
179	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
180	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

#	Article	IF	Citations
181	Topological Phase Transition in Sb₂Mg₃ Assisted by Strain. ACS Omega, 2019, 4, 8701-8706.	1.6	11
182	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
183	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
184	Intramolecular Singlet Fission in Quinoidal Dihydrothiophene. Journal of Physical Chemistry C, 2019, 123, 4749-4754.	1.5	10
185	Stability of cyclic (H2O)n clusters within molecular solids: Role of aromaticity. International Journal of Quantum Chemistry, 2006, 106, 1697-1702.	1.0	9
186	Regioâ€•and stereoselective synthesis of 1â€benzopyrano[2,3â€•b]pyrrolo[2,3â€•d]pyridines: A microwaveâ€•accelerated intramolecular [3+2] cycloaddition reaction of azomethine ylide. Journal of Heterocyclic Chemistry, 2011, 48, 763-768.	1.4	9
187	Synthesis, structure, photocatalytic and magnetic properties of an oxo-bridged copper dimer. RSC Advances, 2014, 4, 21195-21200.	1.7	9
188	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
189	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
190	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
191	Tuning intermediate adsorption in structurally ordered substituted PdCu3 intermetallic nanoparticles for enhanced ethanol oxidation reaction. Chemical Communications, 2021, 57, 4508-4511.	2.2	9
192	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
193	Heavy-atom tunneling in organic transformations. Journal of Chemical Sciences, 2020, 132, 1.	0.7	8
194	Metalâ€free Kinugasa reaction catalyzed by external electric field. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	8
195	Li and Be clusters: Structure, bonding and odd-even effects in half-filled systems. Computing Letters, 2005, 1, 271-276.	0.5	6
196	Formation of Metallic Polyferrocene Chains under Pressure. Journal of Physical Chemistry A, 2021, 125, 3362-3368.	1.1	6
197	An NHCâ€Stabilised Phosphinidene for Catalytic Formylation: A DFTâ€Guided Approach. Chemistry - A European Journal, 2021, 27, 11656-11662.	1.7	6
198	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

#	Article	IF	Citations
199	Molecular modelling of a chemodosimeter for the selective detection of As(III) ion in water. Journal of Chemical Sciences, 2008, 120, 627-635.	0.7	5
200	Ï€-Stacking interactions between G-quartets and circulenes: A computational study. Journal of Chemical Sciences, 2011, 123, 891-900.	0.7	5
201	Pronounced Tunneling Effect of Proton Transfer in Thiotropolone at Room Temperature: A Reply. Angewandte Chemie - International Edition, 2013, 52, 8206-8207.	7.2	5
202	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
203	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
204	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
205	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
206	Stereoelectronic and dynamical effects dictate nitrogen inversion during valence isomerism in benzene imine. Chemical Science, 2022, 13, 704-712.	3.7	5
207	Tunnelling effects in chemistry. Resonance, 2014, 19, 160-174.	0.2	4
208	A Solution Processed Ultrathin Molecular Dielectric for Organic Field-Effect Transistors. ACS Applied Electronic Materials, 2019, 1, 485-493.	2.0	4
209	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
210	Understanding Peierls distortion in one-dimensional infinite V-chain and Vâ€“Bz multi-decker complex. Chemical Physics Letters, 2009, 479, 133-136.	1.2	3
211	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
212	Adsorbate-Induced Phase Transformation of Ambient Stable Noncubic Lattices in Au Microcrystallites. Journal of Physical Chemistry C, 2022, 126, 823-831.	1.5	3
213	Copper Nanoclusters for Catalytic Carbonâ€“Carbon and Carbonâ€“Nitrogen Bond Formations. ACS Applied Nano Materials, 0, , .	2.4	3
214	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
215	Proton-pump mechanism in retinal Schiff base: On the molecular structure of the M-state. Synthetic Metals, 2005, 155, 402-405.	2.1	2
216	Effects of Charging on the Structural and Electronic Properties of Aun Nanoclusters (n = 2-20). , 2011, , .		2

#	Article	IF	Citations
217	A Vision on Organosilicon Chemistry and Silicene. Nanoscience and Technology, 2018, , 1-21.	1.5	2
218	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
219	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
220	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
221	A Hierarchical (Macro)molecular Assembly Assisted by Donorâ€Acceptor Chargeâ€Transfer Interactions Exhibiting Roomâ€Temperature Ferroelectricity. Angewandte Chemie, 0, , .	1.6	2
222	Epitaxial Orientation Angle Tuned Disk-on-Rod Nanoheterostructures for Boosting Charge Transfer. Journal of Physical Chemistry Letters, 2022, 13, 3804-3811.	2.1	2
223	Thiazole Containing PNA Mimic Regulates c-MYC Gene Expression through DNA G-Quadruplex. Bioconjugate Chemistry, 2022, 33, 1145-1155.	1.8	2
224	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
225	Isophlorin derivatives: Structures and materials for n-Channel Organic Semiconductors. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 203-218.	0.1	1
226	Frontispiece: Goldâ€Catalyzed Crossâ€Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. Chemistry - A European Journal, 2020, 26, .	1.7	1
227	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
228	Compression Produces a Square-Planar Iron Tetracarbonyl. Inorganic Chemistry, 2022, 61, 9055-9062.	1.9	1
229	Charge-Transfer Induced Large Nonlinear Optical Properties of Small Al Clusters: Al4M4 (M: Li, Na, and) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0
230	New Examples of Metalloaromatic Al-Clusters: (Al4M4)Fe(CO)3 (M: Li, Na and K) and (Al4M4)2Ni: Rationalization for Possible Synthesis.. ChemInform, 2006, 37, no.	0.1	0
231	Classroom. Resonance, 2016, 21, 377-379.	0.2	0
232	Cobalt phthalocyanine (CoPc) monolayer: A computational study on oxygen reduction reaction (ORR). AIP Conference Proceedings, 2020, , .	0.3	0