# 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 | Structures and Chemical Properties of Silicene: Unlike Graphene. Accounts of Chemical Research, 2014, 47, 593-602. | 15.6 | 291 |
| 2 | Dipolar interactions and hydrogen bonding in supramolecular aggregates: understanding cooperative phenomena for 1st hyperpolarizability. Chemical Society Reviews, 2006, 35, 1305. | 38.1 | 227 |
| 3 | Understanding of the Buckling Distortions in Silicene. Journal of Physical Chemistry C, 2012, 116, 24639-24648. | 3.1 | 188 |
| 4 | Monolayer Group IVâ€“VI Monochalcogenides: Low-Dimensional Materials for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2017, 121, 7615-7624. | 3.1 | 154 |
| 5 | A Thiadiazole-Based Covalent Organic Framework: A Metal-Free Electrocatalyst toward Oxygen Evolution Reaction. ACS Catalysis, 2020, 10, 5623-5630. | 11.2 | 140 |
| 6 | Goldâ€Catalyzed Crossâ€Coupling Reactions: An Overview of Design Strategies, Mechanistic Studies, and Applications. Chemistry - A European Journal, 2020, 26, 1442-1487. | 3.3 | 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. | 17.4 | 126 |
| 8 | Structures and electronic properties of silicene clusters: a promising material for FET and hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 7304. | 2.8 | 125 |
| 9 | Electronic and Chemical Properties of Germanene: The Crucial Role of Buckling. Journal of Physical Chemistry C, 2015, 119, 3802-3809. | 3.1 | 125 |
| 10 | Two-Dimensional Group IV Monochalcogenides: Anode Materials for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 14522-14530. | 3.1 | 120 |
| 11 | Dipole orientation effects on nonlinear optical properties of organic molecular aggregates. Journal of Chemical Physics, 2003, 118, 8420-8427. | 3.0 | 117 |
| 12 | Experimental Evidence for Heavy-Atom Tunneling in the Ring-Opening of Cyclopropylcarbinyl Radical from Intramolecular <sup>12</sup>C/<sup>13</sup>C Kinetic Isotope Effects. Journal of the American Chemical Society, 2010, 132, 12548-12549. | 13.7 | 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. | 13.7 | 81 |
| 14 | Electron and hole mobilities in polymorphs of benzene and naphthalene: Role of intermolecular interactions. Journal of Chemical Physics, 2007, 126, 144710. | 3.0 | 78 |
| 15 | Molecular Balances Based on Aliphatic CHâ‹¯Ï€ and Lone-Pairâ‹¯Ï€ Interactions. Journal of Physical Chemistry Letters, 2012, 3, 1493-1496. | 4.6 | 78 |
| 16 | Highâ€Mobility Field Effect Transistors Based on Supramolecular Charge Transfer Nanofibres. Advanced Materials, 2013, 25, 559-564. | 21.0 | 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. | 4.6 | 73 |
| 18 | Exotic Physics and Chemistry of Two-Dimensional Phosphorus: Phosphorene. Journal of Physical Chemistry Letters, 2017, 8, 2909-2916. | 4.6 | 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 / | 2.5 | 68 |
| 20 | Defects in nanosilica catalytically convert CO <sub>2</sub> to methane without any metal and ligand. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6383-6390. | 7.1 | 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. | 2.6 | 66 |
| 23 | Nucleic Acid G-quartets: Insights into Diverse Patterns and Optical Properties. Journal of Physical Chemistry C, 2011, 115, 12530-12546. | 3.1 | 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. | 2.8 | 64 |
| 25 | Polymorphism Controlled Singlet Fission in TIPS-Anthracene: Role of Stacking Orientation. Journal of Physical Chemistry C, 2017, 121, 1412-1420. | 3.1 | 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. | 3.1 | 59 |
| 27 | Silicon-Doped Nitrogen-Coordinated Graphene as Electrocatalyst for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 27233-27240. | 3.1 | 59 |
| 28 | Remarkable CO<sub>x</sub> tolerance of Ni<sup>3+</sup> active species in a Ni<sub>2</sub>O<sub>3</sub> catalyst for sustained electrochemical urea oxidation. Journal of Materials Chemistry A, 2022, 10, 4209-4221. | 10.3 | 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. | 13.7 | 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. | 13.7 | 56 |
| 31 | Exclusively Ligand-Mediated Catalytic Dehydrogenation of Alcohols. Inorganic Chemistry, 2016, 55, 9602-9610. | 4.0 | 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. | 5.3 | 54 |
| 33 | Designing Molecular Switches Based on DNA-Base Mispairing. Journal of Physical Chemistry B, 2010, 114, 15311-15318. | 2.6 | 54 |
| 34 | Controlled Pore Sizes in Monolayer C<sub>2</sub>N Act as Ultrasensitive Probes for Detection of Gaseous Pollutants (HF, HCN, and H<sub>2</sub>S). Journal of Physical Chemistry C, 2018, 122, 2248-2258. | 3.1 | 53 |
| 35 | Preparation of multi-coloured different sized fluorescent gold clusters from blue to NIR, structural analysis of the blue emitting Au<sub>7</sub>cluster, and cell-imaging by the NIR gold cluster. Nanoscale, 2015, 7, 1912-1920. | 5.6 | 51 |
| 36 | Metalâ€Free Reduction of CO<sub>2</sub> to Methoxyborane under Ambient Conditions through Borondiformate Formation. Angewandte Chemie - International Edition, 2016, 55, 15147-15151. | 13.8 | 50 |

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| 37 | Nonlocal Electronic Distribution in Metallic Clusters:â€‰ A Critical Examination of Aromatic Stabilization. Accounts of Chemical Research, 2007, 40, 213-221. | 15.6 | 49 |
| 38 | Nanoparticle-Catalyzed Clock Reaction. Journal of Physical Chemistry C, 2008, 112, 3619-3626. | 3.1 | 49 |
| 39 | Effect of External Electric Field on Hâ€Bonding and Ïâ€Stacking Interactions in Guanine Aggregates. ChemPhysChem, 2012, 13, 4163-4172. | 2.1 | 48 |
| 40 | A charge transfer single crystal field effect transistor operating at low voltages. Chemical Communications, 2013, 49, 5847. | 4.1 | 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. | 3.3 | 48 |
| 42 | Computational Design of High Hydrogen Adsorption Efficiency in Molecular â€œSulflowerâ€• Journal of Physical Chemistry C, 2007, 111, 4487-4490. | 3.1 | 47 |
| 43 | Role of Metal Ions (M = Li<sup>+</sup>, Na<sup>+</sup>, and K<sup>+</sup>) and Pore Sizes (Crown-4,) Tj ETQq1 1 0.784314 rgBT /O Birefringence. Journal of Physical Chemistry C, 2009, 113, 3339-3344. | 3.1 | 47 |
| 44 | External electric field control: driving the reactivity of metal-free azideâ€“alkyne click reactions. Physical Chemistry Chemical Physics, 2017, 19, 22482-22486. | 2.8 | 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. | 3.1 | 46 |
| 46 | Red-Emitting Copper Nanoclusters: From Bulk-Scale Synthesis to Catalytic Reduction. ACS Sustainable Chemistry and Engineering, 2019, 7, 1998-2007. | 6.7 | 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. | 3.0 | 45 |
| 48 | Role of Multicentered Bonding in Controlling Magnetic Interactions in Ï€-Stacked Bis-dithiazolyl Radical. Crystal Growth and Design, 2011, 11, 3137-3140. | 3.0 | 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. | 4.0 | 45 |
| 50 | Computational design of concomitant type-I and type-II porphyrin sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 18471. | 2.8 | 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. | 3.3 | 44 |
| 52 | Ultrafast Relaxation Dynamics of Luminescent Copper Nanoclusters (Cu<sub>7</sub>L<sub>3</sub>) and Efficient Electron Transfer to Functionalized Reduced Graphene Oxide. Journal of Physical Chemistry C, 2018, 122, 13354-13362. | 3.1 | 44 |
| 53 | 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 |
| 54 | Ordering and Dynamics for the Formation of Two-Dimensional Molecular Crystals on Black Phosphorene. Journal of Physical Chemistry C, 2017, 121, 10210-10223. | 3.1 | 43 |

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| 55 | Design and Applications of Noncanonical DNA Base Pairs. Journal of Physical Chemistry Letters, 2014, 5, 154-166. | 4.6 | 41 |
| 56 | Phenalenyl in a Different Role: Catalytic Activation through the Nonbonding Molecular Orbital. ACS Catalysis, 2014, 4, 4307-4319. | 11.2 | 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. | 2.8 | 40 |
| 58 | Gauging the Nanotoxicity of h2D-C<sub>2</sub>N toward Single-Stranded DNA: An in Silico Molecular Simulation Approach. ACS Applied Materials & Interfaces, 2018, 10, 13805-13818. | 8.0 | 39 |
| 59 | Do Cationâ‹…â‹…â‹…Ï€ Interactions Always Need to be 1:1?. ChemPhysChem, 2012, 13, 695-698. | 2.1 | 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. | 2.6 | 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. | 4.0 | 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. | 13.8 | 36 |
| 64 | What Sustains the Unnatural Base Pairs (UBPs) with No Hydrogen Bonds. Journal of Physical Chemistry B, 2015, 119, 5839-5845. | 2.6 | 36 |
| 65 | Small Organic Molecules for Efficient Singlet Fission: Role of Silicon Substitution. Journal of Physical Chemistry C, 2015, 119, 25696-25702. | 3.1 | 36 |
| 66 | Nonlinear Optical Properties in Calix[n]arenes: Orientation Effects of Monomers. Chemistry - A European Journal, 2005, 11, 4961-4969. | 3.3 | 35 |
| 67 | Noble-Metal-Supported GeS Monolayer as Promising Single-Atom Catalyst for CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 14488-14498. | 3.1 | 35 |
| 68 | Structures and Electronic Properties of Si-Substituted Benzenes and Their Transition-Metal Complexes. Journal of Physical Chemistry Letters, 2010, 1, 136-140. | 4.6 | 34 |
| 69 | Cooperative Interactions in Supramolecular Aggregates: Linear and Nonlinear Responses in Calix[4]arenes. ChemPhysChem, 2006, 7, 2168-2174. | 2.1 | 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. | 3.1 | 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. | 3.1 | 33 |
| 72 | Phase Coexistence and Strain-Induced Topological Insulator in Two-Dimensional BiAs. Journal of Physical Chemistry C, 2018, 122, 15047-15054. | 3.1 | 33 |

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|---|---|---|---|
| 73 | Aromaticity in Stable Tiara Nickel Thiolates:â€‰ Computational and Structural Analysis. Journal of Physical Chemistry A, 2005, 109, 11647-11649. | 2.5 | 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. | 13.7 | 32 |
| 75 | Size specific emission in peptide capped gold quantum clusters with tunable photoswitching behavior. Nanoscale, 2017, 9, 4419-4429. | 5.6 | 32 |
| 76 | Topochemical Transformations of CaX<sub>2</sub> (X=C, Si, Ge) to Form Freeâ€Standing Twoâ€Dimensional Materials. Chemistry - A European Journal, 2015, 21, 18454-18460. | 3.3 | 31 |
| 77 | Direct and Autocatalytic Reductive Elimination from Gold Complexes ([(Ph<sub>3</sub>P)Au(Ar)(CF<sub>3</sub>)(X)], X=F, Cl, Br, I): The Key Role of Halide Ligands. Chemistry - A European Journal, 2017, 23, 4169-4179. | 3.3 | 31 |
| 78 | Magnetic Interactions in Layered Nickel Alkanethiolates. Journal of Physical Chemistry C, 2007, 111, 1868-1870. | 3.1 | 30 |
| 79 | What Stabilizes the Li<sub>n</sub>P<sub>n</sub> Inorganic Double Helices?. Journal of Physical Chemistry Letters, 2013, 4, 1018-1022. | 4.6 | 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. | 6.8 | 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. | 2.1 | 29 |
| 82 | Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. Inorganic Chemistry, 2018, 57, 11995-12009. | 4.0 | 29 |
| 83 | Pt/Co<sub>3</sub>O<sub>4</sub> Surpasses Benchmark Pt/C: An Approach Toward Next Generation Hydrogen Evolution Electrocatalyst. ACS Applied Energy Materials, 2019, 2, 5613-5621. | 5.1 | 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. | 13.7 | 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. | 3.1 | 28 |
| 86 | Half-sandwich Ru(Î·<sup>6</sup>-C<sub>6</sub>H<sub>6</sub>) complexes with chiral aroylthioureas for enhanced asymmetric transfer hydrogenation of ketones â€“ experimental and theoretical studies. Catalysis Science and Technology, 2015, 5, 4790-4799. | 4.1 | 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. | 2.8 | 28 |
| 88 | Two-Dimensional Grapheneâ€“Gold Interfaces Serve as Robust Templates for Dielectric Capacitors. ACS Applied Materials & Interfaces, 2017, 9, 34213-34220. | 8.0 | 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. | 2.6 | 27 |

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| 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. | 1.9 | 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. | 2.8 | 27 |
| 93 | Tip enhanced Raman spectroscopy (TERS) as a probe for the buckling distortion in silicene. Physical Chemistry Chemical Physics, 2013, 15, 8700. | 2.8 | 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. | 2.6 | 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. | 2.6 | 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. | 3.1 | 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. | 5.3 | 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. | 3.1 | 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. | 2.6 | 25 |
| 100 | Designing C<sub>6</sub>N<sub>6</sub>/C<sub>2</sub>N van der Waals heterostructures for photogenerated charge carrier separation. Physical Chemistry Chemical Physics, 2021, 23, 3925-3933. | 2.8 | 25 |
| 101 | Direct CO<sub>2</sub> capture and conversion to fuels on magnesium nanoparticles under ambient conditions simply using water. Chemical Science, 2021, 12, 5774-5786. | 7.4 | 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. | 4.1 | 23 |
| 103 | Structure and electronic properties of the Watsonâ€“Crick base pairs: Role of hydrogen bonding. Synthetic Metals, 2005, 155, 398-401. | 3.9 | 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. | 2.6 | 23 |
| 105 | Tunneling Governs Intramolecular Proton Transfer in Thiotropolone at Room Temperature. Angewandte Chemie - International Edition, 2012, 51, 9389-9392. | 13.8 | 23 |
| 106 | Metal Free Azideâ€“Alkyne Click Reaction: Role of Substituents and Heavy Atom Tunneling. Journal of Physical Chemistry B, 2015, 119, 11540-11547. | 2.6 | 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. | 2.8 | 23 |
| 108 | Multifunctional mixed ligand metal organic frameworks: X-ray structure, adsorption, luminescence and electrical conductivity with theoretical correlation. CrystEngComm, 2016, 18, 5754-5763. | 2.6 | 23 |

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|---|---|---|---|
| 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. | 3.2 | 23 |
| 110 | Exploring Ultrashort Hydrogenâ€“Hydrogen Nonbonded Contacts in Constrained Molecular Cavities. Journal of Physical Chemistry B, 2017, 121, 825-834. | 2.6 | 23 |
| 111 | Topological Insulator in Two-Dimensional SiGe Induced by Biaxial Tensile Strain. ACS Omega, 2018, 3, 1-7. | 3.5 | 23 |
| 112 | Evidence of homo-FRET in quantum dotâ€“dye heterostructured assembly. Physical Chemistry Chemical Physics, 2018, 20, 9523-9535. | 2.8 | 23 |
| 113 | Screening two dimensional materials for the transportation and delivery of diverse genetic materials. Nanoscale, 2020, 12, 703-719. | 5.6 | 23 |
| 114 | How Stable are the Mgâˆ’Mg Bonds in Magnesium (I) Compounds toward Hydrogenation?. Journal of Physical Chemistry C, 2008, 112, 18727-18729. | 3.1 | 22 |
| 115 | Molecular Rotor Inside a Phosphonate Cavitand: Role of Supramolecular Interactions. Journal of Physical Chemistry Letters, 2010, 1, 1363-1366. | 4.6 | 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. | 2.5 | 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. | 3.2 | 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. | 3.1 | 22 |
| 119 | Aryl-platform-based tetrapodal 2-iodo-imidazolium as an excellent halogen bond receptor in aqueous medium. Chemical Communications, 2019, 55, 1506-1509. | 4.1 | 22 |
| 120 | Computationally Driven Design Principles for Singlet Fission in Organic Chromophores. Journal of Physical Chemistry C, 2019, 123, 19257-19268. | 3.1 | 22 |
| 121 | Harnessing the Efficacy of 2-Pyridone Ligands for Pd-Catalyzed (Î²/Î³)-C(sp<sup>3</sup>)â€“H Activations. Journal of Organic Chemistry, 2020, 85, 13228-13238. | 3.2 | 22 |
| 122 | Understanding Thermal and Photochemical Arylâ€“Aryl Crossâ€Coupling by the Au<sup>I</sup>/Au<sup>III</sup> Redox Couple. Chemistry - A European Journal, 2018, 24, 13636-13646. | 3.3 | 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. | 2.5 | 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. | 3.0 | 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. | 4.6 | 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 |

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| 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. | 1.5 | 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. | 3.2 | 19 |
| 129 | Transforming atmospheric CO<sub>2</sub> into alternative fuels: a metal-free approach under ambient conditions. Chemical Science, 2019, 10, 1879-1884. | 7.4 | 19 |
| 130 | Nickelâ€“cobalt oxalate as an efficient non-precious electrocatalyst for an improved alkaline oxygen evolution reaction. Nanoscale Advances, 2021, 3, 3770-3779. | 4.6 | 19 |
| 131 | Hierarchical Structures in Tin(II) Oxalates. European Journal of Inorganic Chemistry, 2008, 2008, 1376-1385. | 2.0 | 18 |
| 132 | Strain Control: Reversible H<sub>2</sub> Activation and H<sub>2</sub>/D<sub>2</sub> Exchange in Pt Complexes. Inorganic Chemistry, 2016, 55, 3023-3029. | 4.0 | 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. | 3.1 | 18 |
| 134 | Novel Brâ‹…â‹…â‹…Ï€(Chelate) Interaction in a 1D Coordination Polymer Revealing Aromaticity. ChemistrySelect, 2018, 3, 4289-4291. | 1.5 | 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. | 13.7 | 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. | 2.6 | 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. | 3.1 | 17 |
| 138 | Disentangling the liquid phase exfoliation of two-dimensional materials: an â€œin silicoâ€• perspective. Physical Chemistry Chemical Physics, 2020, 22, 22157-22179. | 2.8 | 17 |
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