Ankan Paul

List of Publications by Year
in descending order

57	1,623	361296	302012
papers	citations	20 h-index	39 g-index

66	66	66	1631
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Role of Copper Salts and O₂in the Mechanism of Câ‰¡N Bond Activation for Facilitating Nitrogen Transfer Reactions**. Angewandte Chemie, 2022, 134, .	1.6	0
2	The curious saga of dehydrogenation/hydrogenation for chemical hydrogen storage: a mechanistic perspective. Chemical Communications, 2022, 58, 1672-1684.	2.2	7
3	The Role of Copper Salts and O 2 in the Mechanism of Câ‰¡N Bond Activation for Facilitating Nitrogen Transfer Reactions**. Angewandte Chemie - International Edition, 2022, , .	7.2	2
4	Room-Temperature Synthesis of 1,3,5-Tri(het)aryl Benzene from Nitroalkenes Using Pd(OAc)₂: Complete Mechanistic and Theoretical Studies. Organic Letters, 2022, 24, 4438-4443.	2.4	5
5	Unraveling the stability of cyclobutadiene complexes using aromaticity markers. Physical Chemistry Chemical Physics, 2021, 23, 16005-16012.	1.3	6
6	Externally Regulated Specific Molecular Recognition Driven Pathway Selectivity in Supramolecular Polymerization. Chemistry - A European Journal, 2021, 27, 11458-11467.	1.7	7
7	Frustrated Lewis Acidâ€“Base-Pair-Catalyzed Amine-Borane Dehydrogenation. Inorganic Chemistry, 2020, 59, 1046-1056.	1.9	17
8	Computational Investigation of the Mechanism of FLP Catalyzed H₂Activation and Lewis Base Assisted Proton Transfer. ChemistrySelect, 2020, 5, 13397-13406.	0.7	5
9	Comprehending the quadruple bonding conundrum in C₂ from excited state potential energy curves. Chemical Science, 2020, 11, 7009-7014.	3.7	6
10	Understanding the Role of Aromaticity and Conformational Changes in Bond Dissociation Processes of Photo-Protecting Groups. Journal of Physical Chemistry A, 2020, 124, 3976-3983.	1.1	7
11	Atomic layer deposition of amorphous antimony sulfide (a-Sb2S3) as semiconductor sensitizer in extremely thin absorber solar cell. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, 032407.	0.9	6
12	Atomic Layer Deposition of an Sb₂Se₃ Photoabsorber Layer Using Selenium Dimethyldithiocarbamate as a New Se Precursor. Chemistry of Materials, 2019, 31, 7434-7442.	3.2	28
13	Understanding the Role of Solvents and Spinâ€“Orbit Coupling in an Oxygenâ€Assisted S N 2â€Type Oxidative Transmetalation Reaction. Chemistry - A European Journal, 2019, 25, 16606-16616.	1.7	2
14	Exploring the Crucial Role of Solvation on the Viability of Sustainable Hydrogen Storage in BN-fullerene: A Combined DFT and Ab Initio Molecular Dynamics Investigation. ACS Sustainable Chemistry and Engineering, 2019, 7, 9808-9821.	3.2	15
15	Designing Efficient Solar-Thermal Fuels with [n.n](9,10)Anthracene Cyclophanes: A Theoretical Perspective. Journal of Physical Chemistry Letters, 2018, 9, 328-334.	2.1	20
16	Theoretical Investigations on the Mechanistic Aspects of O₂ Activation by a Biomimetic Dinitrosyl Iron Complex. Chemistry - A European Journal, 2018, 24, 3330-3339.	1.7	16
17	Understanding the Unexpected Product Distribution in the Aerial Oxidation of Carbeneâ€Stabilized Diphosphorus Complex. Chemistry - A European Journal, 2018, 24, 4350-4360.	1.7	4
18	Unraveling the Crucial Role of Single Active Water Molecule in the Oxidative Cleavage of Aliphatic Câ€“C Bond of 2,4â€²-Dihydroxyacetophenone Catalyzed by 2,4â€²-Dihydroxyacetophenone Dioxygenase Enzyme: A Quantum Mechanics/Molecular Mechanics Investigation. ACS Catalysis, 2018, 8, 10043-10050.	5.5	26

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19	Unraveling the Microscopic Origin of Triplet Lasing from Organic Solids. Journal of Physical Chemistry Letters, 2018, 9, 4314-4318.	2.1	9
20	Designing an Effective Metalâ€Free Lewis Acid Catalyst for Ammoniaâ€Borane Dehydrogenation: A DFT Investigation on Triarylboranes. ChemCatChem, 2017, 9, 3870-3879.	1.8	13
21	Photochemical Hydrogenation of CO₂ to CH₃OH and Pyridine to 1,2-Dihydropyridine Using Plasmon-Facilitated Chemisorbed Hydrogen on Au Surface: Theoretical Perspective. Journal of Physical Chemistry C, 2017, 121, 15326-15332.	1.5	10
22	Lewis Acid Promoted Hydrogenation of CO₂ and HCOO^{â€“} by Amine Boranes: Mechanistic Insight from a Computational Approach. Journal of Physical Chemistry A, 2017, 121, 5204-5216.	1.1	16
23	A Serendipitous Rendezvous with a Fourâ€Center Twoâ€Electron Bonded Intermediate in the Aerial Oxidation of Hydrazine. Chemistry - A European Journal, 2016, 22, 1216-1222.	1.7	6
24	In Pursuit of Sustainable Hydrogen Storage with Boronâ€Nitride Fullerene as the Storage Medium. ChemSusChem, 2016, 9, 1386-1391.	3.6	18
25	Mechanistic Details of Ruâ€“Bis(pyridyl)borate Complex Catalyzed Dehydrogenation of Ammoniaâ€“Borane: Role of the Pendant Boron Ligand in Catalysis. ACS Catalysis, 2016, 6, 4068-4080.	5.5	20
26	Combining Protons and Hydrides by Homogeneous Catalysis for Controlling the Release of Hydrogen from Ammoniaâ€“Borane: Present Status and Challenges. ACS Catalysis, 2016, 6, 7907-7934.	5.5	103
27	Deciphering the cryptic role of a catalytic electron in a photochemical bond dissociation using excited state aromaticity markers. Physical Chemistry Chemical Physics, 2016, 18, 25308-25314.	1.3	14
28	Rational Design for Complementary Donorâ€“Acceptor Recognition Pairs Using Selfâ€Complementary Hydrogen Bonds. Chemistry - A European Journal, 2016, 22, 1908-1913.	1.7	18
29	Frontispiece: A Serendipitous Rendezvous with a Fourâ€Center Twoâ€Electron Bonded Intermediate in the Aerial Oxidation of Hydrazine. Chemistry - A European Journal, 2016, 22, .	1.7	0
30	Frontispiece: Rational Design for Complementary Donorâ€“Acceptor Recognition Pairs Using Selfâ€Complementary Hydrogen Bonds. Chemistry - A European Journal, 2016, 22, .	1.7	0
31	Theoretical Investigation on the Chemistry of Entrapment of the Elusive Aminoborane (H₂Nï£¾BH₂) Molecule. Chemistry - A European Journal, 2015, 21, 6340-6345.	1.7	16
32	Frontispiece: Theoretical Investigation on the Chemistry of Entrapment of the Elusive Aminoborane (H2Nï£¾BH2) Molecule. Chemistry - A European Journal, 2015, 21, n/a-n/a.	1.7	0
33	Computational design of an Iridium based catalyst for releasing H₂ from hydrogenated BN nanotubes. Chemical Communications, 2015, 51, 10532-10535.	2.2	11
34	Theoretical Studies on the Mechanism of Homogeneous Catalytic Olefin Hydrogenation and Amineâ€“Borane Dehydrogenation by a Versatile Boryl-Ligand-Based Cobalt Catalyst. ACS Catalysis, 2015, 5, 2754-2769.	5.5	55
35	Unraveling the Crucial Role of Metal-Free Catalysis in Borazine and Polyborazylene Formation in Transition-Metal-Catalyzed Ammoniaâ€“Borane Dehydrogenation. ACS Catalysis, 2015, 5, 3478-3493.	5.5	47
36	SeD radical as a probe for the measurement of the time variation of the fine-structure constantÎ±and proton-to-electron mass ratioÎ¼. Physical Review A, 2014, 90, .	1.0	4

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37	Unearthing the Mechanism of Prebiotic Nitrile Bond Reduction in Hydrogen Cyanide through a Curious Association of Two Molecular Radical Anions. Chemistry - A European Journal, 2014, 20, 6348-6357.	1.7	11
38	Reactivity of Biomimetic Iron(II)-2-aminophenolate Complexes toward Dioxygen: Mechanistic Investigations on the Oxidative Câ€“C Bond Cleavage of Substituted 2-Aminophenols. Inorganic Chemistry, 2014, 53, 4899-4912.	1.9	32
39	Unfolding the crucial role of a nucleophile in Zieglerâ€“Natta type Ir catalyzed polyaminoborane formation. Chemical Communications, 2014, 50, 5919.	2.2	38
40	Dramatic reduction in the activation barrier for dinitrogen splitting using amineâ€“borane as a hydrogen carrier: insights from the DFT study. Chemical Communications, 2014, 50, 2187.	2.2	4
41	A Metalâ€Free Strategy to Release Chemisorbed H₂ from Hydrogenated Boron Nitride Nanotubes. Angewandte Chemie - International Edition, 2014, 53, 12430-12435.	7.2	9
42	Selfâ€Assembly of Carboxylic Acid Appended Naphthalene Diimide Derivatives with Tunable Luminescent Color and Electrical Conductivity. Chemistry - A European Journal, 2014, 20, 760-771.	1.7	98
43	Theoretical Insights on the Effects of Mechanical Interlocking of Secondary Amines with Polyether Macrocycles for Frustratedâ€Lewisâ€Pairâ€Type Hydrogen Activation. Chemistry - A European Journal, 2013, 19, 11541-11546.	1.7	7
44	The Role of Solvent and of Species Generated in Situ on the Kinetic Acceleration of Aminoborane Oligomerization. Chemistry - A European Journal, 2013, 19, 5812-5817.	1.7	34
45	Ammoniaâ€“Borane Dehydrogenation by Means of an Unexpected Pentacoordinate Boron Species: Insights from Density Functional and Molecular Dynamics Studies. Chemistry - A European Journal, 2013, 19, 17673-17678.	1.7	13
46	Breaking the Myth of the Recalcitrant Chemisorbed Hydrogens on Boron Nitride Nanotubes: A Theoretical Perspective. Angewandte Chemie - International Edition, 2012, 51, 4152-4156.	7.2	22
47	Changing Lanes from Concerted to Stepwise Hydrogenation: The Reduction Mechanism of Frustrated Lewis Acidâ€“Base Pair Trapped CO₂ to Methanol by Ammoniaâ€“Borane. Chemistry - A European Journal, 2011, 17, 435-439.	1.7	48
48	Hydrogenâ€Bonding Directed Assembly and Gelation of Donorâ€“Acceptor Chromophores: Supramolecular Reorganization from a Chargeâ€Transfer State to a Selfâ€Sorted State. Chemistry - A European Journal, 2011, 17, 6061-6066.	1.7	64
49	The Role of Free Nâ€Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammoniaâ€“Borane in the Nickel NHC System. Angewandte Chemie - International Edition, 2009, 48, 2201-2205.	7.2	115
50	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâˆ'Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	1.9	108
51	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. Inorganic Chemistry, 2009, 48, 5418-5433.	1.9	72
52	Coupled cluster investigation on the low-lying electronic states of CuCN and CuNC and the ground state barrier to isomerization. Journal of Chemical Physics, 2007, 127, 154324.	1.2	6
53	A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cisplatin and Catalytica. Organometallics, 2007, 26, 793-809.	1.1	49
54	Catalyzed Dehydrogenation of Ammoniaâ€“Borane by Iridium Dihydrogen Pincer Complex Differs from Ethane Dehydrogenation. Angewandte Chemie - International Edition, 2007, 46, 8153-8156.	7.2	194

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55	High electron affinities of bicyclo[n,n, 0]perfluoroalkanes. Molecular Physics, 2006, 104, 1311-1324.	0.8	3
56	The low-lying electronic states of nickel cyanide and isocyanide: A theoretical investigation. Journal of Chemical Physics, 2006, 124, 034310.	1.2	15
57	The Peculiar Trend of Cyclic Perfluoroalkane Electron Affinities with Increasing Ring Size. Journal of the American Chemical Society, 2005, 127, 15457-15469.	6.6	29