Gaurab Ganguly

List of Publications by Year
in descending order

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Version: 2024-02-01

43	1,279	471371	360920
papers	citations	17 h-index	35 g-index

47	47	47	1217
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâˆ’Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	1.9	108
4	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
5	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. Inorganic Chemistry, 2009, 48, 5418-5433.	1.9	72
6	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
7	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
8	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
9	Unfolding the crucial role of a nucleophile in Zieglerâ€“Natta type Ir catalyzed polyaminoborane formation. Chemical Communications, 2014, 50, 5919.	2.2	38
10	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
11	A Mononuclear Nonheme Iron(IV)-Oxo Complex of a Substituted N4Py Ligand: Effect of Ligand Field on Oxygen Atom Transfer and Câ€“H Bond Cleavage Reactivity. Inorganic Chemistry, 2019, 58, 1862-1876.	1.9	32
12	Ab Initio Analysis of Metalâ€“Ligand Bonding in An(COT)₂ with An=Th, U in Their Groundâ€and Coreâ€Excited States. Chemistry - A European Journal, 2020, 26, 1776-1788.	1.7	23
13	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
14	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
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	In Pursuit of Sustainable Hydrogen Storage with Boronâ€Nitride Fullerene as the Storage Medium. ChemSusChem, 2016, 9, 1386-1391.	3.6	18
17	Frustrated Lewis Acidâ€“Base-Pair-Catalyzed Amine-Borane Dehydrogenation. Inorganic Chemistry, 2020, 59, 1046-1056.	1.9	17
18	Theoretical Investigation on the Chemistry of Entrapment of the Elusive Aminoborane (H₂Ni£¾BH₂) Molecule. Chemistry - A European Journal, 2015, 21, 6340-6345.	1.7	16

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19	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
20	Insight into the Electronic Structure of Formal Lanthanide(II) Complexes using Magnetic Circular Dichroism Spectroscopy. Organometallics, 2019, 38, 3124-3131.	1.1	16
21	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
22	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
23	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
24	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
25	Mono- and dinuclear oxidovanadium(<scp>v</scp>) complexes of an amine-bis(phenolate) ligand with bromo-peroxidase activities: synthesis, characterization, catalytic, kinetic and computational studies. Dalton Transactions, 2018, 47, 2799-2809.	1.6	12
26	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
27	Computational design of an Iridium based catalyst for releasing H₂ from hydrogenated BN nanotubes. Chemical Communications, 2015, 51, 10532-10535.	2.2	11
28	Cisâ€“Trans Conformational Analysis of Î´-Azaproline in Peptides. Journal of Organic Chemistry, 2015, 80, 10585-10604.	1.7	11
29	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
30	Enhanced 5f-Î´ bonding in [U(C7H7)2]â^': C K-edge XAS, magnetism, and ab initio calculations. Chemical Communications, 2021, 57, 9562-9565.	2.2	10
31	A Metalâ€Free Strategy to Release Chemisorbed H₂ from Hydrogenated Boron Nitride Nanotubes. Angewandte Chemie - International Edition, 2014, 53, 12430-12435.	7.2	9
32	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
33	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
34	The curious saga of dehydrogenation/hydrogenation for chemical hydrogen storage: a mechanistic perspective. Chemical Communications, 2022, 58, 1672-1684.	2.2	7
35	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
36	Unraveling the stability of cyclobutadiene complexes using aromaticity markers. Physical Chemistry Chemical Physics, 2021, 23, 16005-16012.	1.3	6

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37	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
38	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
39	A Benzooxazoleâ€Based Probe for the Sensitive Detection of Hydrogen Sulfide: Kinetic and Transitionâ€State Studies and In Vitro Application in HepG2 Cells. ChemistrySelect, 2018, 3, 7283-7290.	0.7	4
40	Ab Initio Study of Vibronic and Magnetic 5f-to-5f and Dipole-Allowed 5f-to-6d and Charge-Transfer Transitions in [UX₆]^{nâ^'} (X = Cl, Br; n = 1, 2). Journal of Chemical Theory and Computation, 2020, 16, 5189-5202.	2.3	4
41	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
42	Near-infrared C-term MCD spectroscopy of octahedral uranium(<scp>v</scp>) complexes. Dalton Transactions, 2021, 50, 5483-5492.	1.6	2
43	Frontispiece: Ab Initio Analysis of Metalâ€“Ligand Bonding in An(COT)₂ with An=Th, U in Their Groundâ€and Coreâ€Excited States. Chemistry - A European Journal, 2020, 26, .	1.7	0