Bhaskar Mondal

List of Publications by Year
in descending order

43	1,272	471509 17	361022 35
papers	citations	h-index	g-index

45	45	45	1724
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electrocatalytic Water Oxidation Activity of Molecular Copper Complexes: Effect of Redox-Active Ligands. Inorganic Chemistry, 2022, 61, 3152-3165.	4.0	14
2	Absorption and emission of light in red emissive carbon nanodots. Chemical Science, 2021, 12, 3615-3626.	7.4	86
3	Molecular-level insights into the self-assembly driven enantioselective recognition process. Chemical Communications, 2021, 57, 2535-2538.	4.1	6
4	Hidden ligand noninnocence: A combined spectroscopic and computational perspective. Coordination Chemistry Reviews, 2020, 405, 213115.	18.8	20
5	Computational mechanistic insights into non-noble-metal-catalysed CO₂ conversion. Dalton Transactions, 2020, 49, 16608-16616.	3.3	4
6	Orthogonal Selectivity in Câ€“H Olefination: Synthesis of Branched Vinylarene with Unactivated Aliphatic Substitution. ACS Catalysis, 2019, 9, 9606-9613.	11.2	30
7	Reduction of CO₂ by a masked two-coordinate cobalt(<scp>i</scp>) complex and characterization of a proposed oxodicobalt(<scp>ii</scp>) intermediate. Chemical Science, 2019, 10, 918-929.	7.4	44
8	Electron Paramagnetic Resonance Signature of Tetragonal Low Spin Iron(V)-Nitrido and -Oxo Complexes Derived from the Electronic Structure Analysis of Heme and Non-Heme Archetypes. Journal of the American Chemical Society, 2019, 141, 2421-2434.	13.7	45
9	Electronic Structure Contributions of Non-Heme Oxo-Iron(V) Complexes to the Reactivity. Journal of the American Chemical Society, 2018, 140, 9531-9544.	13.7	72
10	Nonclassical Single-State Reactivity of an Oxo-Iron(IV) Complex Confined to Triplet Pathways. Journal of the American Chemical Society, 2017, 139, 8939-8949.	13.7	87
11	Toward Rational Design of 3d Transition Metal Catalysts for CO₂ Hydrogenation Based on Insights into Hydricity-Controlled Rate-Determining Steps. Inorganic Chemistry, 2016, 55, 5438-5444.	4.0	71
12	Magnetic Circular Dichroism Evidence for an Unusual Electronic Structure of a Tetracarbeneâ€“Oxoiron(IV) Complex. Journal of the American Chemical Society, 2016, 138, 14312-14325.	13.7	52
13	Highâ€Valent Ironâ€Oxo and â€Nitrido Complexes: Bonding and Reactivity. Israel Journal of Chemistry, 2016, 56, 763-772.	2.3	32
14	Bio-inspired mechanistic insights into CO2 reduction. Current Opinion in Chemical Biology, 2015, 25, 103-109.	6.1	88
15	Control in the Rate-Determining Step Provides a Promising Strategy To Develop New Catalysts for CO₂ Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study. Inorganic Chemistry, 2015, 54, 7192-7198.	4.0	85
16	The Synthesis of Highly Active Iridium(I) Complexes and their Application in Catalytic Hydrogen Isotope Exchange. Advanced Synthesis and Catalysis, 2014, 356, 3551-3562.	4.3	107
17	Organic super-electron-donors: initiators in transition metal-free haloareneâ€“arene coupling. Chemical Science, 2014, 5, 476-482.	7.4	149
18	Towards a quantitative understanding of palladium metal scavenger performance: an electronic structure calculation approach. Dalton Transactions, 2014, 43, 469-478.	3.3	10

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19	Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes. Organic and Biomolecular Chemistry, 2014, 12, 3598-3603.	2.8	55
20	Overturning Established Chemoselectivities: Selective Reduction of Arenes over Malonates and Cyanoacetates by Photoactivated Organic Electron Donors. Journal of the American Chemical Society, 2013, 135, 10934-10937.	13.7	67
21	Association reaction between SiH3 and H2O2: a computational study of the reaction mechanism and kinetics. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	7
22	Binding affinity of substituted ureidoâ€benzenesulfonamide ligands to the carbonic anhydrase receptor: A theoretical study of enzyme inhibition. Journal of Computational Chemistry, 2013, 34, 1907-1916.	3.3	5
23	Nucleophilic Degradation of Fenitrothion Insecticide and Performance of Nucleophiles: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 2536-2546.	2.5	23
24	Theoretical study of spectroscopy, interaction, and dissociation of linear and T-shaped isomers of RgClF (RgÂ=ÂHe, Ne, and Ar) van der Waals complexes. Structural Chemistry, 2012, 23, 681-692.	2.0	8
25	The association reaction between C2H and 1-butyne: a computational chemical kinetics study. Physical Chemistry Chemical Physics, 2011, 13, 4583.	2.8	7
26	Pyrolysis oftert-Butyltert-Butanethiosulfinate,t-BuS(O)St-Bu: A Computational Perspective of the Decomposition Pathways. Journal of Physical Chemistry A, 2011, 115, 3068-3078.	2.5	7
27	Structure, stability and energetics of ionic arsenicâ€“water complexes. Molecular Physics, 2011, 109, 933-941.	1.7	2
28	Theoretical study of [Si,O,C,O] species: Prediction of new species on triplet potential energy surface. International Journal of Quantum Chemistry, 2011, 111, 606-615.	2.0	0
29	Spectroscopic properties of I2â€“Rg (Rg=He, Ne, Ar) van der Waals complexes. Chemical Physics Letters, 2011, 505, 81-86.	2.6	15
30	Computational study on the doublet [H,S,Si,O] isomers: Structure, stability and dissociation. Computational and Theoretical Chemistry, 2010, 955, 78-83.	1.5	0
31	Structure, stability and dissociation of silanitriles RSiN (RÂ=ÂH2B, H2N, H2P). Structural Chemistry, 2010, 21, 947-954.	2.0	3
32	Structure and dissociation of cyanogen halides BrCN and ICN. International Journal of Quantum Chemistry, 2010, 110, 1165-1171.	2.0	4
33	Computational Study on the Growth of Gallium Nitride and a Possible Source of Oxygen Impurity. Journal of Physical Chemistry A, 2010, 114, 5016-5025.	2.5	10
34	Isomerization and Decomposition of a Model Nerve Agent: A Computational Analysis of the Reaction Energetics and Kinetics of Dimethyl Ethylphosphonate. Journal of Physical Chemistry A, 2010, 114, 10717-10725.	2.5	17
35	Isomers of OCS and their reaction with H₂O on singlet potential energy surface. Molecular Physics, 2010, 108, 3353-3364.	1.7	3
36	Arsine and its fluoro, chloro derivatives: a computational thermochemical study. Molecular Physics, 2010, 108, 1-11.	1.7	11

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37	Spectroscopy and dissociation of sulfuryl halides SO₂X₂(X=F, Cl). Molecular Physics, 2009, 107, 1811-1816.	1.7	1
38	Potential energy surface and thermochemistry for the direct gas phase reaction of germane and water. Structural Chemistry, 2009, 20, 851-858.	2.0	3
39	Stability, spectroscopic constants, and dissociation of CO²⁺: A theoretical study. International Journal of Quantum Chemistry, 2009, 109, 469-476.	2.0	4
40	New molecular species of potential interest to interstellar chemistry: A theoretical study of MgSiN, MgNSi and related species. Chemical Physics, 2009, 364, 105-110.	1.9	0
41	Theoretical study of spectroscopy and dissociation of SO2Br2 and SO2I2. Chemical Physics Letters, 2009, 477, 28-31.	2.6	1
42	Thermochemistry for silicic acid formation reaction: Prediction of new reaction pathway. Chemical Physics Letters, 2009, 478, 115-119.	2.6	16
43	Dissociation and thermochemistry of methylsilanitrile and silylsilanitrile: implications for the chemistry of silicon in interstellar medium. Molecular Physics, 2009, 107, 157-164.	1.7	0