

Debasish Mandal

List of Publications by Year in descending order

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57
papers

2,226
citations

236612

25
h-index

223531

46
g-index

58
all docs

58
docs citations

58
times ranked

2589
citing authors

#	ARTICLE	IF	CITATIONS
1	Oriented electric fields as future smart reagents in chemistry. <i>Nature Chemistry</i> , 2016, 8, 1091-1098.	6.6	391
2	Structure and reactivity/selectivity control by oriented-external electric fields. <i>Chemical Society Reviews</i> , 2018, 47, 5125-5145.	18.7	292
3	How Does Tunneling Contribute to Counterintuitive H-Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes?. <i>Journal of the American Chemical Society</i> , 2015, 137, 722-733.	6.6	89
4	Interplay of Experiment and Theory in Elucidating Mechanisms of Oxidation Reactions by a Nonheme Ru ^{IV} O Complex. <i>Journal of the American Chemical Society</i> , 2015, 137, 8623-8632.	6.6	85
5	Interplay of Tunneling, Two-State Reactivity, and Bell-Evans-Polanyi Effects in C-H Activation by Nonheme Fe(IV)O Oxidants. <i>Journal of the American Chemical Society</i> , 2016, 138, 2094-2097.	6.6	76
6	Kinetic Isotope Effect Determination Probes the Spin of the Transition State, Its Stereochemistry, and Its Ligand Sphere in Hydrogen Abstraction Reactions of Oxoiron(IV) Complexes. <i>Accounts of Chemical Research</i> , 2018, 51, 107-117.	7.6	75
7	Highly Sensitive and Selective Rhodamine-Based Reversible Chemosensor for Tin (Sn ⁴⁺) and Imaging in Living Cells. <i>Inorganic Chemistry</i> , 2013, 52, 10825-10834.	1.9	68
8	Ratiometric sensing of fluoride and acetate anions based on a BODIPY-azaindole platform and its application to living cell imaging. <i>Analyst</i> , 2014, 139, 309-317.	1.7	68
9	A cyclization-induced emission enhancement (CIEE)-based ratiometric fluorogenic and chromogenic probe for the facile detection of a nerve agent simulant DCP. <i>Chemical Communications</i> , 2015, 51, 9729-9732.	2.2	66
10	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold-Thiolate Linkers Innocent?. <i>Journal of the American Chemical Society</i> , 2018, 140, 4354-4362.	6.6	66
11	Determination of Spin Inversion Probability, H-Tunneling Correction, and Regioselectivity in the Two-State Reactivity of Nonheme Iron(IV)-Oxo Complexes. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1472-1476.	2.1	64
12	Emergence of Function in P450-Proteins: A Combined Quantum Mechanical/Molecular Mechanical and Molecular Dynamics Study of the Reactive Species in the H ₂ O ₂ -Dependent Cytochrome P450 ^{SPI±} and Its Regio- and Enantioselective Hydroxylation of Fatty Acids. <i>Journal of the American Chemical Society</i> , 2016, 138, 6786-6797.	6.6	54
13	A BODIPY/pyrene-based chemodosimetric fluorescent chemosensor for selective sensing of hydrazine in the gas and aqueous solution state and its imaging in living cells. <i>RSC Advances</i> , 2015, 5, 58228-58236.	1.7	46
14	Kinetics and Mechanism of the Tropospheric Oxidation of Vinyl Acetate Initiated by OH Radical: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3739-3750.	1.1	44
15	A simple Schiff base molecular logic gate for detection of Zn ²⁺ in water and its bio-imaging application in plant system. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 321, 99-109.	2.0	42
16	Simple Bisthiocarbonohydrazone as a Sensitive, Selective, Colorimetric, and Ratiometric Fluorescent Chemosensor for Picric Acids. <i>ACS Omega</i> , 2017, 2, 1583-1593.	1.6	42
17	Pyrophosphate-selective fluorescent chemosensor based on ratiometric tripod-al-Zn(II) complex: Application in logic gates and living cells. <i>Sensors and Actuators B: Chemical</i> , 2014, 200, 123-131.	4.0	40
18	Colorimetric and ratiometric fluorescent chemodosimeter for selective sensing of fluoride and cyanide ions: tuning selectivity in proton transfer and C-Si bond cleavage. <i>RSC Advances</i> , 2015, 5, 10716-10722.	1.7	39

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19	An azodyeâ€“rhodamine-based fluorescent and colorimetric probe specific for the detection of Pd ²⁺ in aqueous ethanolic solution: synthesis, XRD characterization, computational studies and imaging in live cells. <i>Analyst</i> , 2015, 140, 1229-1236.	1.7	36
20	Benzthiazole-derived chromogenic, fluorogenic and ratiometric probes for detection of hydrazine in environmental samples and living cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 334, 1-12.	2.0	36
21	A chromogenic and ratiometric fluorogenic probe for rapid detection of a nerve agent simulant DCP based on a hybrid hydroxynaphthaleneâ€“hemicyanine dye. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 5959-5967.	1.5	34
22	Privileged Role of Thiolate as the Axial Ligand in Hydrogen Atom Transfer Reactions by Oxoiron(IV) Complexes in Shaping the Potential Energy Surface and Inducing Significant H-Atom Tunneling. <i>Journal of the American Chemical Society</i> , 2017, 139, 18705-18713.	6.6	33
23	Oxoiron(IV) Complex of the Ethylene-Bridged Dialkylcyclam Ligand Me ₂ EBC. <i>Inorganic Chemistry</i> , 2015, 54, 7828-7839.	1.9	28
24	Colorimetric and ratiometric fluorescent chemosensor for fluoride ions based on phenanthroimidazole (PI): spectroscopic, NMR and density functional studies. <i>RSC Advances</i> , 2015, 5, 37935-37942.	1.7	27
25	Structure and spin state of nonheme Fe ^{IV} O complexes depending on temperature: predictive insights from DFT calculations and experiments. <i>Chemical Science</i> , 2017, 8, 5460-5467.	3.7	25
26	A turn-on fluorescent and colorimetric chemodosimeter for selective detection of Au ³⁺ ions in solution and in live cells via Au ³⁺ -induced hydrolysis of a rhodamine-derived Schiff base. <i>New Journal of Chemistry</i> , 2020, 44, 7954-7961.	1.4	25
27	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. <i>Inorganic Chemistry</i> , 2017, 56, 3287-3301.	1.9	24
28	Nucleophilic Degradation of Fenitrothion Insecticide and Performance of Nucleophiles: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2536-2546.	1.1	23
29	Fluorescence sensing of caffeine in aqueous solution with carbazole-based probe and imaging application in live cells. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 5379-5383.	1.0	20
30	Reaction-based bi-signaling chemodosimeter probe for selective detection of hydrogen sulfide and cellular studies. <i>New Journal of Chemistry</i> , 2018, 42, 5367-5375.	1.4	19
31	Aminolysis of a Model Nerve Agent: A Computational Reaction Mechanism Study of O,S-Dimethyl Methylphosphonothiolate. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8382-8396.	1.1	18
32	Carbazole phenylthiosemicarbazone-based ensemble of Hg ²⁺ as selective fluorescence turn-on sensor toward cysteine in water. <i>Tetrahedron Letters</i> , 2013, 54, 2946-2951.	0.7	18
33	Isomerization and Decomposition of a Model Nerve Agent: A Computational Analysis of the Reaction Energetics and Kinetics of Dimethyl Ethylphosphonate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10717-10725.	1.1	17
34	A pyrene thiazole conjugate as a ratiometric chemosensor with high selectivity and sensitivity for tin (Sn ⁴⁺) and its application in imaging live cells. <i>RSC Advances</i> , 2014, 4, 56605-56614.	1.7	16
35	A Michael additionâ€“cyclization-based switch-on fluorescent chemodosimeter for cysteine and its application in live cell imaging. <i>New Journal of Chemistry</i> , 2018, 42, 4951-4958.	1.4	16
36	Interaction Between Group IIb Divalent Transition-Metal Cations and 3-Mercaptopropionic Acid: A Computational and Topological Perspective. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1601-1613.	1.1	15

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37	A benzopyrylium-phenothiazine conjugate of a flavylum derivative as a fluorescent chemosensor for cyanide in aqueous media and its bioimaging. <i>New Journal of Chemistry</i> , 2017, 41, 12581-12588.	1.4	15
38	“Turn-on” fluorescence sensing of cytosine: development of a chemosensor for quantification of cytosine in human cancer cells. <i>RSC Advances</i> , 2017, 7, 54008-54012.	1.7	15
39	Reaction-based ratiometric fluorescent probe for selective recognition of sulfide anions with a large Stokes shift through switching on ESIPT. <i>New Journal of Chemistry</i> , 2018, 42, 76-84.	1.4	15
40	A xanthene-based novel colorimetric and fluorometric chemosensor for the detection of hydrazine and its application in the bio-imaging of live cells. <i>New Journal of Chemistry</i> , 2021, 45, 15869-15875.	1.4	11
41	Computational Study on the Growth of Gallium Nitride and a Possible Source of Oxygen Impurity. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5016-5025.	1.1	10
42	Density functional theory study of interaction, bonding and affinity of group IIb transition metal cations with nucleic acid bases. <i>Chemical Physics</i> , 2012, 400, 108-117.	0.9	10
43	Theoretical study of spectroscopy, interaction, and dissociation of linear and T-shaped isomers of RgClF (Rg=He, Ne, and Ar) van der Waals complexes. <i>Structural Chemistry</i> , 2012, 23, 681-692.	1.0	8
44	Reaction-based sensing of fluoride ions using desilylation method for triggering excited-state intramolecular proton transfer. <i>Supramolecular Chemistry</i> , 2016, 28, 693-706.	1.5	8
45	The association reaction between C ₂ H and 1-butyne: a computational chemical kinetics study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4583.	1.3	7
46	Pyrolysis of tert-Butyl tert-Butanethiosulfinate, t-BuS(O)St-Bu: A Computational Perspective of the Decomposition Pathways. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3068-3078.	1.1	7
47	Installation of efficient quenching groups of a fluorescent probe for the specific detection of cysteine and homocysteine over glutathione in solution and imaging of living cells. <i>Supramolecular Chemistry</i> , 2017, 29, 59-68.	1.5	7
48	Hydrolysis versus aminolysis of a potential nerve agent tabun: a computational reaction mechanism study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	7
49	Fabrication of self-assembled nanostructures for intracellular drug delivery from diphenylalanine analogues with rigid or flexible chemical linkers. <i>Nanoscale Advances</i> , 2021, 3, 6176-6190.	2.2	7
50	A reactive primary fluorescence switch-on sensor for Hg ²⁺ and the generated fluorophore as secondary recognition receptor toward Cu ²⁺ in aqueous acetonitrile solution. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 343, 7-16.	2.0	6
51	A Perylene diimide based fluorescent probe for caffeine in aqueous medium. <i>Supramolecular Chemistry</i> , 2019, 31, 28-35.	1.5	5
52	Mechanism and kinetics for the reaction of O(3P) with DMSO: A theoretical study. <i>Chemical Physics Letters</i> , 2012, 551, 31-37.	1.2	3
53	A Pd-catalyzed one-pot cascade consisting of C-C/O-N bond formation to access benzoxazine fused 1,2,3-triazoles. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9936-9945.	1.5	3
54	Millimeterwave Spectral Studies of Propynal (HCCCHO) Produced by DC Glow Discharge and Ab Initio DFT Calculation. <i>Journal of Atomic, Molecular, and Optical Physics</i> , 2011, 2011, 1-8.	0.5	2

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55	Experimental and Computational Insights into the Water-Mediated Decomposition of N-Sulfonylhydrazones: A Catalyst-Free Synthesis of ^{13}C -Keto/Nitrile Sulfones. Asian Journal of Organic Chemistry, 2020, 9, 251-258.	1.3	1
56	The role of potential energy surface in quantum mechanical tunneling: A computational perspective. Computational and Theoretical Chemistry, 2020, 1187, 112920.	1.1	1
57	Effect of Substituent on C-H Activation Catalysed by a nonheme Fe(IV)O Complex: A Computational Investigation of Reactivity and Hydrogen Tunneling. Dalton Transactions, 0, , .	1.6	1