Tapta Kanchan Roy

List of Publications by Year
in descending order

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38 papers	989 citations	394421 19 h-index	434195 31 g-index
41 all docs	41 docs citations	41 times ranked	1283 citing authors

#	Article	IF	Citations
1	Performance of Vibrational Self-Consistent Field Theory for Accurate Potential Energy Surfaces: Fundamentals, Excited States, and Intensities. Journal of Physical Chemistry A, 2022, 126, 608-622.	2.5	6
2	Effects of non-local exchange functionals in the density functional theories for the description of molecular vibrations. Journal of Chemical Sciences, 2022, 134, .	1.5	2
3	Halloysite Nanotubes Functionalized Sulfonic Acid: Synthesis, Spectroscopic Characterization, Computational Studies and Application for the Synthesis of 1,4-Dihydropyridines. Letters in Organic Chemistry, 2021, 18, .	0.5	6
4	Design, synthesis, characterization and evaluation of the anticancer activity of water-soluble half-sandwich ruthenium(<scp>ii</scp>) arene halido complexes. New Journal of Chemistry, 2020, 44, 239-257.	2.8	37
5	Dual Basis Approach for Ab Initio Anharmonic Calculations of Vibrational Spectroscopy: Application to Microsolvated Biomolecules. Journal of Chemical Theory and Computation, 2020, 16, 7005-7016.	5.3	8
6	Comprehensive Benchmark Results for the Accuracy of Basis Sets for Anharmonic Molecular Vibrations. Journal of Physical Chemistry A, 2020, 124, 9203-9221.	2.5	23
7	On the Proton Shuttle Motion in Protonated Acetylene: An Electronic Structure Perspective. ChemistrySelect, 2020, 5, 9288-9295.	1.5	0
8	Dinuclear gold(I)â€Nâ€heterocyclic carbene complexes: Synthesis, characterization, and catalytic application for hydrohydrazidation of terminal alkynes. Applied Organometallic Chemistry, 2020, 34, e5942.	3.5	3
9	Rhodium(III)â€Catalyzed Annulation of 2â€Arylimidazo[1,2â€a]pyridines with Maleimides: Synthesis of 1Hâ€Benzo[e]pyrido[1â€²,2â€²:1,2]imidazo[4,5â€g]isoindoleâ€1,3(2H)â€Diones and their Photophysical Studies. Advanced Synthesis and Catalysis, 2020, 362, 5751-5764.	4.3	24
10	Comprehensive Analysis of Band Gap and Nanotwinning in Cd_{1â€“x}Mg_xS QDs. Crystal Growth and Design, 2020, 20, 6699-6706.	3.0	8
11	Conjugated small organic molecules: synthesis and characterization of 4-arylpyrazole-decorated dibenzothiophenes. New Journal of Chemistry, 2020, 44, 8944-8951.	2.8	4
12	Novel Axially Ligated Complexes of Zn(II)Porphyrin: Spectroscopic, Computational, and Antibiological Characterization. Russian Journal of Inorganic Chemistry, 2019, 64, 1379-1395.	1.3	3
13	Hypochloriteâ€Mediated Modulation of Photoinduced Electron Transfer in a Phenothiazineâ€“Boron dipyrromethene Electron Donorâ€“Acceptor Dyad: A Highly Water Soluble â€œTurnâ€Onâ€Fluorescent Probe for Hypochlorite. Chemistry - an Asian Journal, 2018, 13, 1594-1608.	3.3	25
14	Synthesis of Diverse Nitrogen Heterocycles via Palladiumâ€Catalyzed Tandem Azideâ€“Isocyanide Crossâ€Coupling/Cyclization: Mechanistic Insight using Experimental and Theoretical Studies. Advanced Synthesis and Catalysis, 2018, 360, 290-297.	4.3	24
15	Azo-dyes based small bifunctional molecules for metal chelation and controlling amyloid formation. Inorganica Chimica Acta, 2018, 471, 419-429.	2.4	25
16	Catalyst-Controlled Structural Divergence: Selective Intramolecular 7-endo-dig and 6-exo-dig Post-Ugi Cyclization for the Synthesis of Benzoxazepinones and Benzoxazinones. Journal of Organic Chemistry, 2018, 83, 57-68.	3.2	32
17	Intrinsic structure of pentapeptide Leu-enkephalin: geometry optimization and validation by comparison of VSCF-PT2 calculations with cold ion spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 24894-24901.	2.8	18
18	Phosphineâ€Free Bis(Pyrrolyl)pyridine Based NNNâ€Pincer Palladium(II) Complexes as Efficient Catalysts for Suzukiâ€Miyaura Crossâ€Coupling Reactions of Aryl Bromides in Aqueous Medium. ChemistrySelect, 2018, 3, 9469-9475.	1.5	17

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19	Synthesis of Spirooxindoles through Cyclocondensation of Isatin and Cyclic 1,3â€Diones. Journal of Heterocyclic Chemistry, 2018, 55, 1783-1790.	2.6	8
20	Hypochlorite-promoted inhibition of photo-induced electron transfer in phenothiazineâ€“borondipyrromethene donorâ€“acceptor dyad: a cost-effective and metal-free â€œturn-onâ€• fluorescent chemosensor for hypochlorite. New Journal of Chemistry, 2017, 41, 5322-5333.	2.8	30
21	A Decapeptide Hydrated by Two Waters: Conformers Determined by Theory and Validated by Cold Ion Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 9401-9408.	2.5	16
22	A catalyst-free, one-pot multicomponent synthesis of spiro-benzimidazoquinazolinones via a Knoevenagelâ€“Michael-imine pathway: a microwave assisted approach. RSC Advances, 2016, 6, 41897-41906.	3.6	28
23	Ruthenium Catalyzed Intramolecular Câ€“S Coupling Reactions: Synthetic Scope and Mechanistic Insight. Organic Letters, 2016, 18, 356-359.	4.6	68
24	First-principles anharmonic quantum calculations for peptide spectroscopy: VSCF calculations and comparison with experiments. Physical Chemistry Chemical Physics, 2016, 18, 1607-1614.	2.8	32
25	Mechanistic studies of malonic acidâ€mediated in situ acylation. Biopolymers, 2015, 104, 495-505.	2.4	3
26	Conformational Structures of a Decapeptide Validated by First Principles Calculations and Cold Ion Spectroscopy. ChemPhysChem, 2015, 16, 1374-1378.	2.1	28
27	Frontispiz: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie, 2014, 126, n/a-n/a.	2.0	0
28	Frontispiece: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie - International Edition, 2014, 53, n/a-n/a.	13.8	0
29	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	2.5	32
30	A comparative study of independent particle model based approaches for thermal averages. Journal of Chemical Sciences, 2013, 125, 1267-1275.	1.5	1
31	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. Physical Chemistry Chemical Physics, 2013, 15, 9468.	2.8	163
32	MOFâ€FF â€“ A flexible firstâ€principles derived force field for metalâ€organic frameworks. Physica Status Solidi (B): Basic Research, 2013, 250, 1128-1141.	1.5	162
33	Development of a new variational approach for thermal density matrices. Journal of Chemical Physics, 2011, 134, 214110.	3.0	11
34	Functionalization of terminal carbon atoms of hydroxyl terminated polybutadiene by polyazido nitrogen rich molecules. Bulletin of Materials Science, 2011, 34, 745-754.	1.7	30
35	A thermal self-consistent field theory for the calculation of molecular vibrational partition functions. Journal of Chemical Physics, 2009, 131, 114102.	3.0	20
36	Terminal functionalized hydroxylâ€terminated polybutadiene: An energetic binder for propellant. Journal of Applied Polymer Science, 2009, 114, 732-741.	2.6	64

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37	Effective harmonic oscillator description of anharmonic molecular vibrations. Journal of Chemical Sciences, 2009, 121, 805-810.	1.5	22
38	Porphyrin Bearing Phenothiazine Pincers as Hosts for Fullerene Binding via Concave-Convex Complementarity: Synthesis and Complexation Study. New Journal of Chemistry, 0, , .	2.8	3