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	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
2	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
3	Ruthenium Catalyzed Intramolecular Câ€“S Coupling Reactions: Synthetic Scope and Mechanistic Insight. Organic Letters, 2016, 18, 356-359.	4.6	68
4	Terminal functionalized hydroxylâ€terminated polybutadiene: An energetic binder for propellant. Journal of Applied Polymer Science, 2009, 114, 732-741.	2.6	64
5	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
6	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
7	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
8	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
9	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
10	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
11	Conformational Structures of a Decapeptide Validated by First Principles Calculations and Cold Ion Spectroscopy. ChemPhysChem, 2015, 16, 1374-1378.	2.1	28
12	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
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	Azo-dyes based small bifunctional molecules for metal chelation and controlling amyloid formation. Inorganica Chimica Acta, 2018, 471, 419-429.	2.4	25
15	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
16	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
17	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
18	Effective harmonic oscillator description of anharmonic molecular vibrations. Journal of Chemical Sciences, 2009, 121, 805-810.	1.5	22

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19	A thermal self-consistent field theory for the calculation of molecular vibrational partition functions. Journal of Chemical Physics, 2009, 131, 114102.	3.0	20
20	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
21	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
22	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
23	Development of a new variational approach for thermal density matrices. Journal of Chemical Physics, 2011, 134, 214110.	3.0	11
24	Synthesis of Spirooxindoles through Cyclocondensation of Isatin and Cyclic 1,3â€Diones. Journal of Heterocyclic Chemistry, 2018, 55, 1783-1790.	2.6	8
25	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
26	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
27	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
28	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
29	Conjugated small organic molecules: synthesis and characterization of 4-arylpyrazole-decorated dibenzothiophenes. New Journal of Chemistry, 2020, 44, 8944-8951.	2.8	4
30	Mechanistic studies of malonic acidâ€mediated in situ acylation. Biopolymers, 2015, 104, 495-505.	2.4	3
31	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
32	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
33	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
34	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
35	A comparative study of independent particle model based approaches for thermal averages. Journal of Chemical Sciences, 2013, 125, 1267-1275.	1.5	1
36	Frontispiz: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie, 2014, 126, n/a-n/a.	2.0	0

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37	Frontispiece: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie - International Edition, 2014, 53, n/a-n/a.	13.8	0
38	On the Proton Shuttle Motion in Protonated Acetylene: An Electronic Structure Perspective. ChemistrySelect, 2020, 5, 9288-9295.	1.5	0