Sanyasi Sitha

List of Publications by Year
in descending order

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Version: 2024-02-01

36 papers	473 citations	687363 13 h-index	713466 21 g-index
36 all docs	36 docs citations	36 times ranked	450 citing authors

#	Article	IF	Citations
1	Enhanced Nonlinear Optical Response in Zwitterionic Molecules:â€‰ A Computational Study on the Role of Orbital Interactions through Ïƒ Bonds. Journal of Physical Chemistry A, 2001, 105, 8727-8733.	2.5	45
2	Near-Infrared Absorption in Symmetric Squarylium and Croconate Dyes:Â A Comparative Study Using Symmetry-Adapted Cluster-Configuration Interaction Methods. Journal of Physical Chemistry A, 2005, 109, 8604-8616.	2.5	45
3	Role of the Oxyallyl Substructure in the Near Infrared (NIR) Absorption in Symmetrical Dye Derivatives:Â A Computational Study. Journal of Physical Chemistry A, 2005, 109, 2614-2622.	2.5	40
4	First hyperpolarizability of some nonconjugated donorâ€“acceptor 3D molecules: noncentrosymmetric crystal through conformational flexibility. Journal of Materials Chemistry, 2005, 15, 965-973.	6.7	33
5	Second-order nonlinear response in mono- and di-substituted triazine derivatives: A combined experimental and theoretical analysis. Optical Materials, 2006, 28, 1006-1012.	3.6	31
6	NLO Activity in some non-conjugated 3D triazine derivatives: a non-centrosymmetric crystal through conformational flexibility. Journal of Materials Chemistry, 2006, 16, 496-504.	6.7	26
7	Possible interstellar formation of glycine through a concerted mechanism: a computational study on the reaction of CH₂î€NH, CO₂ and H₂. Physical Chemistry Chemical Physics, 2016, 18, 20109-20117.	2.8	24
8	Possible interstellar formation of glycine from the reaction of CH₂î€NH, CO and H₂O: catalysis by extra water molecules through the hydrogen relay transport. Physical Chemistry Chemical Physics, 2016, 18, 375-381.	2.8	24
9	Linear allenic linkage for nonlinear optics: A computational study of the role of mutually orthogonal Ï€-orbitals in controlling the charge transfer, hyperpolarizability and absorption properties in some donorâ€“acceptor substituted allenes. Computational and Theoretical Chemistry, 2005, 728, 57-65.	1.5	22
10	Role of aromatic Ï€-bridge on electron transport property in a donorâ€“bridgeâ€“acceptor system: A computational study on frontier molecular orbitals. Computational and Theoretical Chemistry, 2006, 761, 31-38.	1.5	17
11	Electrical rectification through cumulenic bridge: a computational study. Synthetic Metals, 2005, 148, 227-235.	3.9	14
12	Tautomerism of bis(2,4-benzyloxy)-6-(5H)-one-1,3,5-triazine: A combined crystallographic and quantum-chemical investigation. Structural Chemistry, 2006, 17, 561-568.	2.0	14
13	Reaction between HN and SN: a possible channel for the interstellar formation of N₂ and SH in the cold interstellar clouds. Physical Chemistry Chemical Physics, 2015, 17, 32455-32463.	2.8	14
14	Formation of Formamide from HCN + H₂O: A Computational Study on the Roles of a Second H₂O as a Catalyst, as a Spectator, and as a Reactant. Journal of Physical Chemistry A, 2020, 124, 165-175.	2.5	14
15	Efficient discrimination of natural stereoisomers of chicoric acid, an HIV-1 integrase inhibitor. Journal of Photochemistry and Photobiology B: Biology, 2018, 189, 258-266.	3.8	13
16	Reaction between NH₃ (XÌŒ¹A₁) and CO (X¹Î£⁺): A Computational Insight into the Reaction Mechanism of Formamide (H₂Nâ€“CHO) Formation. Journal of Physical Chemistry A, 2019, 123, 8921-8931.	2.5	13
17	Enhanced molecular first hyperpolarizability in s-triazine derivatives: Combined experimental and computational studies. Journal of Molecular Structure, 2014, 1075, 118-123.	3.6	11
18	Expanding the applicability of electrostatic potentials to the realm of transition states. Physical Chemistry Chemical Physics, 2016, 18, 13002-13009.	2.8	11

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19	Roles of various bridges on intramolecular charge Transfers, dipole moments and first hyperpolarizabilities of Donor-Bridge-Acceptor types of organic Chromophores: Theoretical assessment using Two-State model. Computational and Theoretical Chemistry, 2022, 1209, 113583.	2.5	10
20	Non-catalytic hydroamination of alkenes: a computational study. Tetrahedron, 2010, 66, 3030-3036.	1.9	9
21	Theoretical assessment of the influences of aromatic bridges on molecular second order nonlinear optical responses of Donor-Bridge-Acceptor types of molecular organic chromophores. Computational and Theoretical Chemistry, 2022, 1207, 113522.	2.5	9
22	Formation of the Silicon Analogues of Isocyanic Acid, HNSiO, and Its Isomers by Neutralâ^'Neutral Reactions of the Fragments:Â A Computational Studyâ€. Journal of Physical Chemistry A, 2003, 107, 11497-11504.	2.5	7
23	Planar in Brooker's mode and twisted in Reichardt's mode: defying the steric forces in biphenyl types of zwitterionic systems through metameric resonance stabilizations. Physical Chemistry Chemical Physics, 2022, 24, 13110-13118.	2.8	7
24	Formation of a pre-reaction hydrogen-bonded complex and its significance in the potential energy surface of the OH + SO2â†' HOSO₂ reaction: A computational study. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750046.	1.8	6
25	Role of large thermal fluctuations and magnesium ions in t-RNA selectivity of the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3947-3951.	7.1	5
26	A computational study on the formations of formamide analogues: Interesting chemistry by silicon analogues. Computational and Theoretical Chemistry, 2021, 1201, 113290.	2.5	2
27	Possible interstellar formation of phosphorus analogue of hydrazoic acid: A computational study on the reaction between HN and PN. Computational and Theoretical Chemistry, 2016, 1078, 129-137.	2.5	1
28	Some possible channels for the N 2 formation and their probable effects on the interstellar elemental nitrogen partitioning: A computational study. Chemical Physics, 2017, 493, 20-31.	1.9	1
29	Change of magnetic behaviour of nitrogenated carbon nanotubes on chlorination/oxidation. International Journal of Nanotechnology, 2017, 14, 356.	0.2	1
30	Hemiaminal route for the formation of interstellar glycine: a computational study. Journal of Molecular Modeling, 2019, 25, 335.	1.8	1
31	Hydrogenations of Isocyanic Acid: A Computational Study on Four Possible Concerted Paths for Formamide Formation. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
32	Tetrel bonding in the realm of transition states favors silicon over Carbon: Role of water as a tetrel spectator in the formation of silaformamide. Computational and Theoretical Chemistry, 2021, 1205, 113456.	2.5	1
33	Breaking the chiral mirror of alanine with dipole moment and oriented electric field: Violations of parity degeneracy and a possible answer to natureâ€™s homochirality. Computational and Theoretical Chemistry, 2021, 1205, 113446.	2.5	1
34	Potential energy surface of the cationâ€“neutral hydroamination reaction: a computational study on the role of an ionâ€“molecule complex in the reaction pathway. Tetrahedron, 2014, 70, 7906-7911.	1.9	0
35	Potential application of compliance constants in predicting the mass spectral fragmentation of metabolites. Rapid Communications in Mass Spectrometry, 2015, 29, 1874-1878.	1.5	0
36	Reactivity of phosphorus mononitride and interstellar formation of molecules containing phospazo linkage: A computational study on the reaction between HSi (X2Î) and PN (X1Î£+). Journal of Theoretical and Computational Chemistry, 2017, 16, 1750075.	1.8	0