Padmabati Mondal

List of Publications by Year
in descending order

17	326	759233 12	888059 17
papers	citations	h-index	g-index

19	19	19	417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Why intermolecular nitric oxide (NO) transfer? Exploring the factors and mechanistic aspects of NO transfer reaction. Chemical Science, 2022, 13, 1706-1714.	7.4	5
2	Multipolar Force Fields for Amide-I Spectroscopy from Conformational Dynamics of the Alanine Trimer. Journal of Physical Chemistry B, 2021, 125, 10928-10938.	2.6	6
3	Impact of the redox state of flavin chromophores on the UVâ€“vis spectra, redox and acidity constants and electron affinities. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 387, 112164.	3.9	21
4	Non-conventional force fields for applications in spectroscopy and chemical reaction dynamics. Journal of Chemical Physics, 2020, 153, 010901.	3.0	20
5	In silico decryption of serotoninâ€“receptor binding: local non-covalent interactions and long-range conformational changes. RSC Advances, 2020, 10, 37995-38003.	3.6	1
6	Theoretical insights into the formation and stability of radical oxygen species in cryptochromes. Physical Chemistry Chemical Physics, 2019, 21, 8874-8882.	2.8	21
7	Free energy simulations for protein ligand binding and stability. Molecular Simulation, 2018, 44, 1044-1061.	2.0	13
8	Solvent Composition Drives the Rebinding Kinetics of Nitric Oxide to Microperoxidase. Scientific Reports, 2018, 8, 5281.	3.3	4
9	Azobenzene as a photoregulator covalently attached to RNA: a quantum mechanics/molecular mechanics-surface hopping dynamics study. Chemical Science, 2018, 9, 4671-4681.	7.4	20
10	Vibrational Stark spectroscopy for assessing ligand-binding strengths in a protein. Physical Chemistry Chemical Physics, 2017, 19, 16131-16143.	2.8	17
11	Reversible Photoswitching of RNA Hybridization at Room Temperature with an Azobenzene Câ€Nucleoside. Chemistry - A European Journal, 2015, 21, 2845-2854.	3.3	59
12	In Search of an Efficient Photoswitch for Functional RNA: Design Principles from a Microscopic Analysis of Azobenzene-linker-RNA Dynamics with Different Linkers. Journal of Physical Chemistry B, 2015, 119, 11275-11286.	2.6	17
13	Infrared Absorption Spectra of Jahnâ€“Teller Systems: Application to the Transition-Metal Trifluorides MnF₃ and NiF₃. Journal of Physical Chemistry A, 2014, 118, 3726-3734.	2.5	7
14	Ab initio study of dynamical E Ã— e Jahn-Teller and spin-orbit coupling effects in the transition-metal trifluorides TiF3, CrF3, and NiF3. Journal of Chemical Physics, 2012, 136, 084308.	3.0	33
15	Effect of Surface Modes on the Six-Dimensional Moleculeâ€“Surface Scattering Dynamics of H₂â€“Cu(100) and D₂â€“Cu(111) Systems. Journal of Physical Chemistry A, 2011, 115, 5256-5273.	2.5	17
16	Jahnâ€“Teller and spinâ€“orbit coupling effects in transition-metal trifluorides. Chemical Physics, 2011, 387, 56-65.	1.9	42
17	A quantum-classical approach to the molecular dynamics of butatriene cation with a realistic model Hamiltonian. Physical Chemistry Chemical Physics, 2008, 10, 6388.	2.8	23