Debashree Ghosh

List of Publications by Year
in descending order

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47	4,030	361413	223800
papers	citations	20 h-index	46 g-index

51	51	51	5034
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational aspects towards understanding the photoprocesses in eumelanin. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1505.	14.6	4
2	Configuration interaction trained by neural networks: Application to model polyaromatic hydrocarbons. Journal of Chemical Physics, 2021, 154, 094117.	3.0	9
3	Electron Attachment to Cytosine: The Role of Water. Journal of Physical Chemistry A, 2021, 125, 4683-4694.	2.5	9
4	Radiationless Decay Processes of an Unnatural DNA Base: Pyrrole 2-Carbaldehyde. Journal of Physical Chemistry A, 2021, 125, 5556-5561.	2.5	1
5	Effect of Dimerization on the Nonradiative Processes of Eumelanin Monomer. Journal of Physical Chemistry B, 2021, 125, 547-556.	2.6	2
6	Data-driven modeling of S â†' S1 excitation energy in the BODIPY chemical space: High-throughput computation, quantum machine learning, and inverse design. Journal of Chemical Physics, 2021, 155, 244102.	3.0	11
7	Lightâ€induced excited spinâ€state trapping in spin crossover model system. International Journal of Quantum Chemistry, 2020, 120, e26122.	2.0	2
8	Charge transfer in DHICA eumelanin-like oligomers: role of hydrogen bonds. Chemical Communications, 2020, 56, 10481-10484.	4.1	8
9	Comprehending the quadruple bonding conundrum in C₂ from excited state potential energy curves. Chemical Science, 2020, 11, 7009-7014.	7.4	6
10	Support Vector Regression-Based Monte Carlo Simulation of Flexible Water Clusters. ACS Omega, 2020, 5, 7065-7073.	3.5	2
11	In the quest for a stable triplet state in small polyaromatic hydrocarbons: an in silico tool for rational design and prediction. Chemical Science, 2019, 10, 9270-9276.	7.4	14
12	Non-radiative decay of an eumelanin monomer: to be or not to be planar. Physical Chemistry Chemical Physics, 2019, 21, 6635-6642.	2.8	10
13	Effect of microsolvation on the non-radiative decay of the eumelanin monomer. Physical Chemistry Chemical Physics, 2019, 21, 26123-26132.	2.8	5
14	Evolutionary algorithm based configuration interaction approach. International Journal of Quantum Chemistry, 2018, 118, e25509.	2.0	11
15	Machine learning prediction of interaction energies in rigid water clusters. Physical Chemistry Chemical Physics, 2018, 20, 22987-22996.	2.8	11
16	Electrostatic Origin of the Red Solvatochromic Shift of DFHBDI in RNA Spinach. Journal of Physical Chemistry B, 2017, 121, 4790-4798.	2.6	8
17	Elucidating the Photoprotection Mechanism of Eumelanin Monomers. Journal of Physical Chemistry B, 2017, 121, 5988-5994.	2.6	14
18	Effect of solvation on the ionization of guanine nucleotide: A hybrid QM/EFP study. Journal of Computational Chemistry, 2017, 38, 2528-2537.	3.3	12

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19	An interaction energy driven biased sampling technique: A faster route to ionization spectra in condensed phase. Journal of Computational Chemistry, 2017, 38, 2248-2257.	3.3	10
20	Unprecedented solvent induced inter-conversion between monomeric and dimeric silyleneâ€“zinc iodide adducts. Dalton Transactions, 2017, 46, 11418-11424.	3.3	11
21	The nature of selenium hydrogen bonding: gas phase spectroscopy and quantum chemistry calculations. Physical Chemistry Chemical Physics, 2017, 19, 24179-24187.	2.8	51
22	Hybrid Equation-of-Motion Coupled-Cluster/Effective Fragment Potential Method: A Route toward Understanding Photoprocesses in the Condensed Phase. Journal of Physical Chemistry A, 2017, 121, 741-752.	2.5	25
23	Multiscale Modelling:Hybrid Quantum Mechanics/Molecular Mechanics as an Example and some Recent Developments. Current Science, 2017, 112, 1455.	0.8	3
24	Effect of Solvation on Electron Detachment and Excitation Energies of a Green Fluorescent Protein Chromophore Variant. Journal of Physical Chemistry B, 2016, 120, 4410-4420.	2.6	21
25	Extension of the Effective Fragment Potential Method to Macromolecules. Journal of Physical Chemistry B, 2016, 120, 6562-6574.	2.6	72
26	The effect of sequence on the ionization of guanine in DNA. Physical Chemistry Chemical Physics, 2016, 18, 6526-6533.	2.8	22
27	Effects of the benzoxazole group on green fluorescent protein chromophore crystal structure and solid state photophysics. Journal of Materials Chemistry C, 2016, 4, 2793-2801.	5.5	21
28	Singletâ€“triplet gaps in polyacenes: a delicate balance between dynamic and static correlations investigated by spinâ€“flip methods. Physical Chemistry Chemical Physics, 2015, 17, 9849-9856.	2.8	53
29	Feasibility of Ionization-Mediated Pathway for Ultraviolet-Induced Melanin Damage. Journal of Physical Chemistry B, 2015, 119, 13288-13293.	2.6	12
30	Spectroscopic and ab initio investigation of 2,6-difluorophenylacetyleneâ€“amine complexes: coexistence of Câ€“Hâ‹¯N and lone-pairâ‹¯Ï€ complexes and intermolecular coulombic decay. Physical Chemistry Chemical Physics, 2015, 17, 434-443.	2.8	14
31	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
32	Perturbative approximation to hybrid equation of motion coupled cluster/effective fragment potential method. Journal of Chemical Physics, 2014, 140, 094101.	3.0	12
33	Electrostatics determine vibrational frequency shifts in hydrogen bonded complexes. Physical Chemistry Chemical Physics, 2014, 16, 25247-25250.	2.8	26
34	Ionization-Induced Tautomerization in Cytosine and Effect of Solvation. Journal of Physical Chemistry A, 2014, 118, 5323-5332.	2.5	10
35	Effective fragment potential method in <scp>Qâ€CHEM</scp>: A guide for users and developers. Journal of Computational Chemistry, 2013, 34, 1060-1070.	3.3	47
36	Perturbative approximations to single and double spin flip equation of motion coupled cluster singles doubles methods. Journal of Chemical Physics, 2013, 139, 124116.	3.0	28

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37	Toward Understanding the Redox Properties of Model Chromophores from the Green Fluorescent Protein Family: An Interplay between Conjugation, Resonance Stabilization, and Solvent Effects. Journal of Physical Chemistry B, 2012, 116, 12398-12405.	2.6	20
38	A VUV Photoionization and Ab Initio Determination of the Ionization Energy of a Gas-Phase Sugar (Deoxyribose). Journal of Physical Chemistry Letters, 2012, 3, 97-101.	4.6	41
39	First-Principle Protocol for Calculating Ionization Energies and Redox Potentials of Solvated Molecules and Ions: Theory and Application to Aqueous Phenol and Phenolate. Journal of Physical Chemistry B, 2012, 116, 7269-7280.	2.6	113
40	What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?. Journal of Physical Chemistry Letters, 2011, 2, 2593-2597.	4.6	23
41	Effect of Solvation on the Vertical Ionization Energy of Thymine: From Microhydration to Bulk. Journal of Physical Chemistry A, 2011, 115, 6028-6038.	2.5	95
42	Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. Journal of Physical Chemistry A, 2010, 114, 12739-12754.	2.5	100
43	A study of cumulant approximations to n-electron valence multireference perturbation theory. Journal of Chemical Physics, 2009, 130, 194107.	3.0	70
44	Accelerating convergence in iterative solution for largeâ€scale complete active space selfâ€consistentâ€field calculations. International Journal of Quantum Chemistry, 2009, 109, 2178-2190.	2.0	84
45	Orbital optimization in the density matrix renormalization group, with applications to polyenes and Î²-carotene. Journal of Chemical Physics, 2008, 128, 144117.	3.0	288
46	An Introduction to the Density Matrix Renormalization Group Ansatz in Quantum Chemistry. Progress in Theoretical Chemistry and Physics, 2008, , 49-65.	0.2	57
47	Substitution enables significant new decay channels for a non-canonical amino acid. Physical Chemistry Chemical Physics, 0, , .	2.8	0