Hugo Gattuso

List of Publications by Year
in descending order

35 papers	764 citations	430754 18 h-index	580701 25 g-index
35 all docs	35 docs citations	35 times ranked	1517 citing authors

#	Article	IF	Citations
1	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	1.7	85
2	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. Journal of Physical Chemistry B, 2016, 120, 3113-3121.	1.2	42
3	Excited-states of a rhenium carbonyl diimine complex: solvation models, spinâ€"orbit coupling, and vibrational sampling effects. Physical Chemistry Chemical Physics, 2017, 19, 27240-27250.	1.3	40
4	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. Nucleic Acids Research, 2016, 44, 8588-8599.	6.5	37
5	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. RSC Advances, 2017, 7, 10992-10999.	1.7	36
6	Quantum Phenomena in Nanomaterials: Coherent Superpositions of Fine Structure States in CdSe Nanocrystals at Room Temperature. Journal of Physical Chemistry C, 2019, 123, 31286-31293.	1.5	31
7	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. Journal of Physical Chemistry Letters, 2016, 7, 3760-3765.	2.1	30
8	Dynamics of the excited-state hydrogen transfer in a (dG)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	3.7	29
9	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	1.8	28
10	Room-Temperature Inter-Dot Coherent Dynamics in Multilayer Quantum Dot Materials. Journal of Physical Chemistry C, 2020, 124, 16222-16231.	1.5	27
11	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. Scientific Reports, 2016, 6, 28480.	1.6	24
12	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	1.3	24
13	Modeling DNA electronic circular dichroism by QM/MM methods and Frenkel Hamiltonian. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	22
14	Nile blue and Nile red optical properties predicted by TD-DFT and CASPT2 methods: static and dynamic solvent effects. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	22
15	QM/MM modeling of Harmane cation fluorescence spectrum in water solution and interacting with DNA. Computational and Theoretical Chemistry, 2014, 1040-1041, 367-372.	1.1	20
16	Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. Physical Chemistry Chemical Physics, 2016, 18, 18598-18606.	1.3	20
17	DNA Photosensitization by an â€œInsiderâ€: Photophysics and Triplet Energy Transfer of 5â€Methylâ€2â€pyrimidone Deoxyribonucleoside. Chemistry - A European Journal, 2015, 21, 11509-11516.	1.7	19
18	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	1.6	19

#	Article	IF	Citations
19	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. Physical Chemistry Chemical Physics, 2017, 19, 23187-23193.	1.3	18
20	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	6.5	17
21	Fluorene-imidazole dyes excited states from first-principles calculationsâ€”Topological insights. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
22	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. Frontiers in Chemistry, 2018, 6, 86.	1.8	16
23	Quantum Device Emulates the Dynamics of Two Coupled Oscillators. Journal of Physical Chemistry Letters, 2020, 11, 6990-6995.	2.1	16
24	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. Journal of Chemical Theory and Computation, 2017, 13, 3290-3296.	2.3	15
25	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	2.2	15
26	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
27	Ultrafast fs coherent excitonic dynamics in CdSe quantum dots assemblies addressed and probed by 2D electronic spectroscopy. Journal of Chemical Physics, 2021, 154, 014301.	1.2	13
28	Coherent Exciton Dynamics in Ensembles of Size-Dispersed CdSe Quantum Dot Dimers Probed via Ultrafast Spectroscopy: A Quantum Computational Study. Applied Sciences (Switzerland), 2020, 10, 1328.	1.3	12
29	Massively parallel classical logic via coherent dynamics of an ensemble of quantum systems with dispersion in size. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21022-21030.	3.3	11
30	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	1.3	10
31	Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. Frontiers in Chemistry, 2015, 3, 67.	1.8	9
32	Absorption Spectroscopy and Photophysics of a Re^Iâ€•dppz Probe for DNAâ€•Mediated Charge Transport. Chemistry - A European Journal, 2018, 24, 14425-14435.	1.7	9
33	Chargeâ€•Transfer versus Chargeâ€•Separated Triplet Excited States of [Re^I(dmp)(CO)₃(His124)(Trp122)]⁺ in Water and in Modified <i>Pseudomonas aeruginosa</i> Azurin Protein. Chemistry - A European Journal, 2019, 25, 2519-2526.	1.7	8
34	Photophysics of the Singlet Oxygen Sensor Green Chromophore: Self-Production of ¹O₂ Explained by Molecular Modeling. Journal of Physical Chemistry B, 2017, 121, 7586-7592.	1.2	7
35	Covalent Cross-Linking as an Enabler for Structural Mass Spectrometry. Analytical Chemistry, 2019, 91, 12808-12818.	3.2	3