

Marco Marazzi

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

65 papers	910 citations	17 h-index	26 g-index
82 ext. papers	1,132 ext. citations	5.1 avg, IF	4.49 L-index

#	Paper	IF	Citations
65	E/Z Photochemical switches: syntheses, properties and applications. <i>RSC Advances</i> , 2013 , 3, 6241	3.7	81
64	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 622-6	6.4	71
63	Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1389-96	6.4	47
62	Reaction dynamics of the chimeric channelrhodopsin C1C2. <i>Scientific Reports</i> , 2017 , 7, 7217	4.9	37
61	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. <i>Journal of Proteome Research</i> , 2020 , 19, 4291-4315	5.6	36
60	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. <i>Chemical Science</i> , 2016 , 7, 3879-3891	9.4	33
59	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 17916-17926	3.8	28
58	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. <i>RSC Advances</i> , 2017 , 7, 10992-10999	3.7	27
57	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 25662-25670	3.6	25
56	Dynamics of the excited-state hydrogen transfer in a (dG)I(dC) homopolymer: intrinsic photostability of DNA. <i>Chemical Science</i> , 2018 , 9, 7902-7911	9.4	24
55	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 7829-36	3.6	22
54	Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 18598-606	3.6	20
53	Nile blue and Nile red optical properties predicted by TD-DFT and CASPT2 methods: static and dynamic solvent effects. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	19
52	Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 425-428	6.4	19
51	Optomechanical Control of Quantum Yield in Trans-Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 3842-3846	16.4	18
50	Toward an Optomechanical Control of Photoswitches by Tuning Their Spectroscopical Properties: Structural and Dynamical Insights into Azobenzene. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 312-23	6.4	18
49	Thermodynamics of the Interaction between the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus-2 and the Receptor of Human Angiotensin-Converting Enzyme 2. Effects of Possible Ligands. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9272-9281	6.4	18

48	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5661-5667	6.4	17
47	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. <i>Scientific Reports</i> , 2016 , 6, 28480	4.9	17
46	Level of Theory and Solvent Effects on DASA Absorption Properties Prediction: Comparing TD-DFT, CASPT2 and NEVPT2. <i>Materials</i> , 2017 , 10,	3.5	16
45	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 23187-23193	3.6	14
44	Modulating nitric oxide release by S-nitrosothiol photocleavage: mechanism and substituent effects. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 7039-49	2.8	14
43	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. <i>Frontiers in Chemistry</i> , 2018 , 6, 86	5	13
42	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. <i>Scientific Reports</i> , 2017 , 7, 8885	4.9	13
41	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2570-2585	6.4	12
40	A biomimetic molecular switch at work: coupling photoisomerization dynamics to peptide structural rearrangement. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 6742-53	3.6	12
39	Allyl amino-thioxanthone derivatives as highly efficient visible light H-donors and co-polymerizable photoinitiators. <i>Polymer Chemistry</i> , 2020 , 11, 4297-4312	4.9	12
38	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3290-3296	6.4	11
37	From Light Absorption to Cyclization: Structure and Solvent Effects in Donor-Acceptor Stenhouse Adducts. <i>ChemPhotoChem</i> , 2019 , 3, 866-873	3.3	11
36	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)(Dmp)(His124)(Trp122)] in azurin: a nonadiabatic dynamics study. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 65	1.9	11
35	Ultrafast dynamics in polycyclic aromatic hydrocarbons: the key case of conical intersections at higher excited states and their role in the photophysics of phenanthrene monomer. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 16981-16988	3.6	11
34	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017 , 73, 544-549	1.8	11
33	Dinuclear Gold(I) Complexes Bearing Alkyl-Bridged Bis(N-heterocyclic carbene) Ligands as Catalysts for Carboxylative Cyclization of Propargylamine: Synthesis, Structure, and Kinetic and Mechanistic Comparison to the Mononuclear Complex [Au(IPr)Cl]. <i>Organometallics</i> , 2020 , 39, 2907-2916	3.8	11
32	Different hydrogen bonding environments of the retinal protonated Schiff base control the photoisomerization in channelrhodopsin-2. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 27501-27509	3.6	11
31	Photophysical Properties of Novel Two-Photon Absorbing Dyes: Assessing Their Possible Use for Singlet Oxygen Generation. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 16315-16324	3.8	11

30	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4530-4540	6.4	10
29	Structural Substituent Effect in the Excitation Energy of a Chromophore: Quantitative Determination and Application to S-Nitrosothiols. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3293-302	6.4	10
28	Insights into the mechanism of photosynthetic H ₂ evolution catalyzed by a heptacoordinate cobalt complex. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 589-599	5.8	10
27	Following a photoinduced reconstructive phase transformation and its influence on the crystal integrity: powder diffraction and theoretical study. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 6738-42	16.4	9
26	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7133-7140	6.4	8
25	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4749-4757	3.6	8
24	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. <i>Photochemical and Photobiological Sciences</i> , 2018 , 17, 323-331	4.2	8
23	Far Red Fluorescent Proteins: Where Is the Limit of the Acylimine Chromophore?. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4228-4240	6.4	7
22	Charge-Transfer versus Charge-Separated Triplet Excited States of [Re (dmp)(CO) (His124)(Trp122)] in Water and in Modified Pseudomonas aeruginosa Azurin Protein. <i>Chemistry - A European Journal</i> , 2019 , 25, 2519-2526	4.8	6
21	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15496-15508	3.6	6
20	Photophysics of the Singlet Oxygen Sensor Green Chromophore: Self-Production of O Explained by Molecular Modeling. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 7586-7592	3.4	6
19	First principles study of photostability within hydrogen-bonded amino acids. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7805-11	3.6	6
18	Definition and determination of the triplet-triplet energy transfer reaction coordinate. <i>Journal of Chemical Physics</i> , 2014 , 140, 034102	3.9	5
17	Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State. <i>ChemPhotoChem</i> , 2019 , 3, 925-932	3.3	4
16	Photostability Mechanisms in Human B-Crystallin: Role of the Tyrosine Corner Unveiled by Quantum Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Methodologies. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1351-9	6.4	4
15	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22957-22971	3.6	4
14	Structure and Dynamics of RNA Guanine Quadruplexes in SARS-CoV-2 Genome. Original Strategies against Emerging Viruses. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10277-10283	6.4	4
13	The role of CO detachment in fungal bioluminescence: thermally excited state induced pathways. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 26787-26795	3.6	4

12	Rationalizing Photo-Triggered Hydrogen Evolution Using Polypyridine Cobalt Complexes: Substituent Effects on Hexadentate Chelating Ligands. <i>ChemSusChem</i> , 2021 , 14, 1874-1885	8.3	4
11	Optomechanical Control of Quantum Yield in Trans-Is Ultrafast Photoisomerization of a Retinal Chromophore Model. <i>Angewandte Chemie</i> , 2017 , 129, 3900-3904	3.6	3
10	Mechanochemical Improvement of Norbornadiene-Based Molecular Solar-Thermal Systems Performance. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 19496-19504	8.3	3
9	On the mechanism of the photocyclization of azadienes. <i>Tetrahedron</i> , 2012 , 68, 730-736	2.4	2
8	Thermal and Mechanochemical Tuning of the Porphyrin Singlet-Triplet Gap for Selective Energy Transfer Processes: A Molecular Dynamics Approach. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5429-5439	6.4	2
7	Following a Photoinduced Reconstructive Phase Transformation and its Influence on the Crystal Integrity: Powder Diffraction and Theoretical Study. <i>Angewandte Chemie</i> , 2014 , 126, 6856-6860	3.6	1
6	Bridge Substitution in DASAs: The Subtle Equilibrium between Photochemical Improvements and Thermal Control*. <i>Chemistry - A European Journal</i> , 2021 , 27, 4420-4429	4.8	1
5	Controlling Antimicrobial Activity of Quinolones Using Visible/NIR Light-Activated BODIPY Photocages. <i>Pharmaceutics</i> , 2022 , 14, 1070	6.4	1
4	Chapter 6. Computational Spectroscopy and Photophysics in Complex Biological Systems: Towards an In Silico Photobiology. <i>RSC Theoretical and Computational Chemistry Series</i> , 2020 , 202-246	1.2	0
3	Design of Improved Molecular Solar-Thermal Systems by Mechanochemistry: The Case of Azobenzene. <i>Advanced Sustainable Systems</i> , 2200097	5.9	0
2	Atomistic-Level Description of the Covalent Inhibition of SARS-CoV-2 Papain-like Protease. <i>International Journal of Molecular Sciences</i> , 2022 , 23, 5855	6.3	0
1	Hijacking of Cellular Functions by Severe Acute Respiratory Syndrome Coronavirus-2. Permeabilization and Polarization of the Host Lipid Membrane by Viroporins.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 4642-4649	6.4	