Marco Marazzi

List of Publications by Year in Descending Order

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	Hijacking of Cellular Functions by Severe Acute Respiratory Syndrome Coronavirus-2. Permeabilization and Polarization of the Host Lipid Membrane by Viroporins.. *Journal of Physical Chemistry Letters*, **2022**, 4642-4649	6.4	
64	Controlling Antimicrobial Activity of Quinolones Using Visible/NIR Light-Activated BODIPY Photocages. *Pharmaceutics*, **2022**, 14, 1070	6.4	1
63	Atomistic-Level Description of the Covalent Inhibition of SARS-CoV-2 Papain-like Protease. *International Journal of Molecular Sciences*, **2022**, 23, 5855	6.3	0
62	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. *Physical Chemistry Chemical Physics*, **2021**, 23, 22957-22971	3.6	4
61	Structure and Dynamics of RNA Guanine Quadruplexes in SARS-CoV-2 Genome. Original Strategies against Emerging Viruses. *Journal of Physical Chemistry Letters*, **2021**, 12, 10277-10283	6.4	4
60	Rationalizing Photo-Triggered Hydrogen Evolution Using Polypyridine Cobalt Complexes: Substituent Effects on Hexadentate Chelating Ligands. *ChemSusChem*, **2021**, 14, 1874-1885	8.3	4
59	Bridge Substitution in DASAs: The Subtle Equilibrium between Photochemical Improvements and Thermal Control*. *Chemistry - A European Journal*, **2021**, 27, 4420-4429	4.8	1
58	Thermal and Mechanochemical Tuning of the Porphyrin Singlet-Triplet Gap for Selective Energy Transfer Processes: A Molecular Dynamics Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 5429-5439	6.4	2
57	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. *Journal of Physical Chemistry Letters*, **2020**, 11, 5661-5667	6.4	17
56	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)(Dmp)(His124)(Trp122)] in azurin: a nonadiabatic dynamics study. *Theoretical Chemistry Accounts*, **2020**, 139, 65	1.9	11
55	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. *Physical Chemistry Chemical Physics*, **2020**, 22, 15496-15508	3.6	6
54	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 4749-4757	3.6	8
53	Chapter 6. Computational Spectroscopy and Photophysics in Complex Biological Systems: Towards an In Silico Photobiology. *RSC Theoretical and Computational Chemistry Series*, **2020**, 202-246	1.2	0
52	Allyl amino-thioxanthone derivatives as highly efficient visible light H-donors and co-polymerizable photoinitiators. *Polymer Chemistry*, **2020**, 11, 4297-4312	4.9	12
51	Insights into the mechanism of photosynthetic H2 evolution catalyzed by a heptacoordinate cobalt complex. *Sustainable Energy and Fuels*, **2020**, 4, 589-599	5.8	10
50	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. *Journal of Physical Chemistry Letters*, **2020**, 11, 9272-9281	6.4	18
49	The role of CO detachment in fungal bioluminescence: thermally excited state induced pathways. *Physical Chemistry Chemical Physics*, **2020**, 22, 26787-26795	3.6	4

48	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]. *Organometallics*, **2020**, 39, 2907-2916	3.8	11
47	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. *Journal of Proteome Research*, **2020**, 19, 4291-4315	5.6	36
46	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. *Journal of Physical Chemistry Letters*, **2019**, 10, 7133-7140	6.4	8
45	Charge-Transfer versus Charge-Separated Triplet Excited States of [Re (dmp)(CO) (His124)(Trp122)] in Water and in Modified Pseudomonas aeruginosa Azurin Protein. *Chemistry - A European Journal*, **2019**, 25, 2519-2526	4.8	6
44	From Light Absorption to Cyclization: Structure and Solvent Effects in Donor-Acceptor Stenhouse Adducts. *ChemPhotoChem*, **2019**, 3, 866-873	3.3	11
43	Far Red Fluorescent Proteins: Where Is the Limit of the Acylimine Chromophore?. *Journal of Chemical Theory and Computation*, **2019**, 15, 4228-4240	6.4	7
42	Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State. *ChemPhotoChem*, **2019**, 3, 925-932	3.3	4
41	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. *Physical Chemistry Chemical Physics*, **2019**, 21, 16981-16988	3.6	11
40	Mechanochemical Improvement of Norbornadiene-Based Molecular Solar Thermal Systems Performance. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 19496-19504	8.3	3
39	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 2570-2585	6.4	12
38	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. *Photochemical and Photobiological Sciences*, **2018**, 17, 323-331	4.2	8
37	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. *Frontiers in Chemistry*, **2018**, 6, 86	5	13
36	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. *Journal of Chemical Theory and Computation*, **2018**, 14, 4530-4540	6.4	10
35	Different hydrogen bonding environments of the retinal protonated Schiff base control the photoisomerization in channelrhodopsin-2. *Physical Chemistry Chemical Physics*, **2018**, 20, 27501-27509	3.6	11
34	Dynamics of the excited-state hydrogen transfer in a (dG)(dC) homopolymer: intrinsic photostability of DNA. *Chemical Science*, **2018**, 9, 7902-7911	9.4	24
33	Photophysical Properties of Novel Two-Photon Absorbing Dyes: Assessing Their Possible Use for Singlet Oxygen Generation. *Journal of Physical Chemistry C*, **2018**, 122, 16315-16324	3.8	11
32	Optomechanical Control of Quantum Yield in Trans-Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie - International Edition*, **2017**, 56, 3842-3846	16.4	18
31	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. *RSC Advances*, **2017**, 7, 10992-10999	3.7	27

30	Optomechanical Control of Quantum Yield in Trans□cis Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie*, **2017**, 129, 3900-3904	3.6	3
29	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3290-3296	6.4	11
28	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. *Physical Chemistry Chemical Physics*, **2017**, 19, 25662-25670	3.6	25
27	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. *Scientific Reports*, **2017**, 7, 8885	4.9	13
26	Photophysics of the Singlet Oxygen Sensor Green Chromophore: Self-Production of O Explained by Molecular Modeling. *Journal of Physical Chemistry B*, **2017**, 121, 7586-7592	3.4	6
25	Reaction dynamics of the chimeric channelrhodopsin C1C2. *Scientific Reports*, **2017**, 7, 7217	4.9	37
24	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. *Physical Chemistry Chemical Physics*, **2017**, 19, 23187-23193	3.6	14
23	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 544-549	1.8	11
22	Level of Theory and Solvent Effects on DASA Absorption Properties Prediction: Comparing TD-DFT, CASPT2 and NEVPT2. *Materials*, **2017**, 10,	3.5	16
21	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. *Journal of Physical Chemistry C*, **2016**, 120, 17916-17926	3.8	28
20	Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 18598-606	3.6	20
19	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. *Chemical Science*, **2016**, 7, 3879-3891	9.4	33
18	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. *Physical Chemistry Chemical Physics*, **2016**, 18, 7829-36	3.6	22
17	A biomimetic molecular switch at work: coupling photoisomerization dynamics to peptide structural rearrangement. *Physical Chemistry Chemical Physics*, **2016**, 18, 6742-53	3.6	12
16	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
15	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	1.9	19
14	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. *Scientific Reports*, **2016**, 6, 28480	4.9	17
13	Toward an Optomechanical Control of Photoswitches by Tuning Their Spectroscopical Properties: Structural and Dynamical Insights into Azobenzene. *Journal of Chemical Theory and Computation*, **2014**, 10, 312-23	6.4	18

List of Publications

12	Following a photoinduced reconstructive phase transformation and its influence on the crystal integrity: powder diffraction and theoretical study. *Angewandte Chemie - International Edition*, **2014**, 53, 6738-42	16.4	9
11	Definition and determination of the triplet-triplet energy transfer reaction coordinate. *Journal of Chemical Physics*, **2014**, 140, 034102	3.9	5
10	Following a Photoinduced Reconstructive Phase Transformation and its Influence on the Crystal Integrity: Powder Diffraction and Theoretical Study. *Angewandte Chemie*, **2014**, 126, 6856-6860	3.6	1
9	E/Z Photochemical switches: syntheses, properties and applications. *RSC Advances*, **2013**, 3, 6241	3.7	81
8	Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors. *Journal of Physical Chemistry Letters*, **2013**, 4, 1389-96	6.4	47
7	On the mechanism of the photocyclization of azadienes. *Tetrahedron*, **2012**, 68, 730-736	2.4	2
6	Modulating nitric oxide release by S-nitrosothiol photocleavage: mechanism and substituent effects. *Journal of Physical Chemistry A*, **2012**, 116, 7039-49	2.8	14
5	Photostability Mechanisms in Human B-Crystallin: Role of the Tyrosine Corner Unveiled by Quantum Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Methodologies. *Journal of Chemical Theory and Computation*, **2012**, 8, 1351-9	6.4	4
4	Structural Substituent Effect in the Excitation Energy of a Chromophore: Quantitative Determination and Application to S-Nitrosothiols. *Journal of Chemical Theory and Computation*, **2012**, 8, 3293-302	6.4	10
3	First principles study of photostability within hydrogen-bonded amino acids. *Physical Chemistry Chemical Physics*, **2011**, 13, 7805-11	3.6	6
2	Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins. *Journal of Physical Chemistry Letters*, **2010**, 1, 425-428	6.4	19
1	Design of Improved Molecular Solar-Thermal Systems by Mechanochemistry: The Case of Azobenzene. *Advanced Sustainable Systems*,2200097	5.9	0