Antonio Monari

List of Publications by Citations

193 papers	3,278 citations	30 h-index	44 g-index
259 ext. papers	3,861 ext. citations	4.2 avg, IF	5.66 L-index

#	Paper	IF	Citations
193	Toward a Quantitative Assessment of Electronic Transitions' Charge-Transfer Character. *Journal of Chemical Theory and Computation*, **2014**, 10, 3896-905	6.4	114
192	New Insight into the Topology of Excited States through Detachment/Attachment Density Matrices-Based Centroids of Charge. *Journal of Chemical Theory and Computation*, **2014**, 10, 3906-14	6.4	102
191	A new record excited state (3)MLCT lifetime for metalorganic iron(ii) complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 12550-6	3.6	99
190	An Iron-Based Photosensitizer with Extended Excited-State Lifetime: Photophysical and Photovoltaic Properties. *European Journal of Inorganic Chemistry*, **2015**, 2015, 2469-2477	2.3	96
189	Theoretical modeling of large molecular systems. Advances in the local self consistent field method for mixed quantum mechanics/molecular mechanics calculations. *Accounts of Chemical Research*, **2013**, 46, 596-603	24.3	92
188	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
187	3,5-Bis(ethynyl)pyridine and 2,6-bis(ethynyl)pyridine spanning two Fe(Cp*)(dppe) units: role of the nitrogen atom on the electronic and magnetic couplings. *Inorganic Chemistry*, **2011**, 50, 12601-22	5.1	62
186	NHC-Based Iron Sensitizers for DSSCs. *Inorganics*, **2018**, 6, 63	2.9	55
185	Lipid Peroxidation in Membranes: The Peroxyl Radical Does Not "Float". *Journal of Physical Chemistry Letters*, **2014**, 5, 1653-8	6.4	55
184	A QM/MM study on the spinach plastocyanin: Redox properties and absorption spectra. *Computational and Theoretical Chemistry*, **2012**, 990, 119-125	2	54
183	Heteroleptic Pyridyl-Carbene Iron Complexes with Tuneable Electronic Properties. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3747-3753	2.3	52
182	Spectral properties of polypyridyl ruthenium complexes intercalated in DNA: theoretical insights into the surrounding effects of [Ru(dppz)(bpy)2]2+. *Physical Chemistry Chemical Physics*, **2012**, 14, 12496-504	3.6	50
181	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. *Molecules*, **2018**, 23,	4.8	49
180	Photophysical properties of ruthenium(II) polypyridyl DNA intercalators: effects of the molecular surroundings investigated by theory. *Chemistry - A European Journal*, **2014**, 20, 12901-9	4.8	48
179	Theoretical study of new ruthenium-based dyes for dye-sensitized solar cells. *Journal of Physical Chemistry A*, **2011**, 115, 3596-603	2.8	45
178	Probing the reactivity of singlet oxygen with purines. *Nucleic Acids Research*, **2016**, 44, 56-62	20.1	44
177	Improved Treatment of Surrounding Effects: UV/vis Absorption Properties of a Solvated Ru(II) Complex. *Journal of Chemical Theory and Computation*, **2012**, 8, 1536-41	6.4	44

176	Theoretical evidence of photo-induced charge transfer from DNA to intercalated ruthenium (II) organometallic complexes. *Chemical Physics Letters*, **2013**, 578, 133-137	2.5	44
175	Understanding DNA under oxidative stress and sensitization: the role of molecular modeling. *Frontiers in Chemistry*, **2015**, 3, 43	5	42
174	Interfacial charge separation and photovoltaic efficiency in Fe(ii)-carbene sensitized solar cells. *Physical Chemistry Chemical Physics*, **2016**, 18, 28069-28081	3.6	41
173	A QM/MM study of the absorption spectrum of harmane in water solution and interacting with DNA: the crucial role of dynamic effects. *Journal of Physical Chemistry B*, **2013**, 117, 4973-80	3.4	41
172	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. *Journal of Physical Chemistry Letters*, **2015**, 6, 576-80	6.4	40
171	Benzophenone and DNA: Evidence for a Double Insertion Mode and Its Spectral Signature. *Journal of Physical Chemistry Letters*, **2013**, 4, 4119-4124	6.4	39
170	Excited-states of a rhenium carbonyl diimine complex: solvation models, spin-orbit coupling, and vibrational sampling effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 27240-27250	3.6	36
169	Interaction of palmatine with DNA: an environmentally controlled phototherapy drug. *Journal of Physical Chemistry B*, **2015**, 119, 410-9	3.4	36
168	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
167	Full configuration interaction study of the metal-insulator transition in model systems: LiN linear chains (N=2,4,6,8). *Journal of Chemical Physics*, **2008**, 128, 024701	3.9	31
166	The problem of interoperability: A common data format for quantum chemistry codes. *International Journal of Quantum Chemistry*, **2007**, 107, 2082-2091	2.1	31
165	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. *Journal of Physical Chemistry B*, **2016**, 120, 3113-21	3.4	30
164	A theoretical study of linear beryllium chains: full configuration interaction. *Journal of Chemical Physics*, **2009**, 130, 024301	3.9	30
163	Theoretical computation of Betain B30 solvatochromism using a Polarizable Continuum Model. *Dyes and Pigments*, **2014**, 100, 24-31	4.6	29
162	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. *Nucleic Acids Research*, **2016**, 44, 8588-8599	20.1	29
161	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. *Journal of Physical Chemistry C*, **2016**, 120, 17916-17926	3.8	28
160	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. *RSC Advances*, **2017**, 7, 10992-10999	3.7	27
159	Detection of Nitroaromatic Explosives Based on Fluorescence Quenching of Silafluorene- and Silole-Containing Polymers: A Time-Dependent Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 23946-23953	3.8	26

158	FORTRAN interface for code interoperability in quantum chemistry: the Q5Cost library. *Journal of Chemical Information and Modeling*, **2007**, 47, 1271-7	6.1	26
157	From Physical Mixtures to Co-Crystals: How the Coformers Can Modify Solubility and Biological Activity of Carbamazepine. *Molecular Pharmaceutics*, **2018**, 15, 268-278	5.6	26
156	Synthesis and Computational Study of a Pyridylcarbene Fe(II) Complex: Unexpected Effects of fac/mer Isomerism in Metal-to-Ligand Triplet Potential Energy Surfaces. *Inorganic Chemistry*, **2018**, 57, 10431-10441	5.1	25
155	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
154	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
153	Iron(ii) complexes with diazinyl-NHC ligands: impact of □deficiency of the azine core on photophysical properties. *Dalton Transactions*, **2019**, 48, 10915-10926	4.3	23
152	A priori modeling of chemical reactions on computational grid platforms: Workflows and data models. *Chemical Physics*, **2012**, 398, 192-198	2.3	23
151	The metal-insulator transition in dimerized H□kel chains. *Journal of Chemical Physics*, **2008**, 129, 134104	3.9	23
150	Impact of the fac/ mer Isomerism on the Excited-State Dynamics of Pyridyl-carbene Fe(II) Complexes. *Inorganic Chemistry*, **2019**, 58, 5069-5081	5.1	22
149	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. *Physical Chemistry Chemical Physics*, **2016**, 18, 7829-36	3.6	22
148	All-organic chromophores for dye-sensitized solar cells: A theoretical study on aggregation. *Dyes and Pigments*, **2014**, 101, 203-211	4.6	21
147	Unveiling the nature of post-linear response Z-vector method for time-dependent density functional theory. *Journal of Chemical Physics*, **2017**, 147, 024108	3.9	21
146	Molecular Dynamics Insights into Polyamine-DNA Binding Modes: Implications for Cross-Link Selectivity. *Chemistry - A European Journal*, **2017**, 23, 12845-12852	4.8	21
145	Ground and excited state properties of new porphyrin based dyads: a combined theoretical and experimental study. *Journal of Physical Chemistry A*, **2012**, 116, 10736-44	2.8	21
144	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. *Journal of Physical Chemistry Letters*, **2016**, 7, 3760-3765	6.4	21
143	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. *Frontiers in Chemistry*, **2018**, 6, 495	5	21
142	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
141	Novel quinoxalinone-based push-pull chromophores with highly sensitive emission and absorption properties towards small structural modifications. *Physical Chemistry Chemical Physics*, **2018**, 20, 21515-21527	3.6	20

140	QM/MM modeling of Harmane cation fluorescence spectrum in water solution and interacting with DNA. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 367-372	2	20
139	Modeling DNA electronic circular dichroism by QM/MM methods and Frenkel Hamiltonian. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	19
138	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
137	New dyads using (metallo)porphyrins as ancillary ligands in polypyridine ruthenium complexes. Synthesis and electronic properties. *Dalton Transactions*, **2012**, 41, 12865-71	4.3	19
136	Full-configuration-interaction study of the metal-insulator transition in a model system: Hn linear chains n=4, 6,16. *International Journal of Quantum Chemistry*, **2011**, 111, 3416-3423	2.1	19
135	Strong delocalization and substitution effect on electronic properties of dithienylpyrrole-containing bipyridine ligands and corresponding ruthenium complexes. *Dalton Transactions*, **2012**, 41, 4833-44	4.3	18
134	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
133	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
132	A FCI benchmark on beryllium dimer: The lowest singlet and triplet states. *Chemical Physics Letters*, **2013**, 568-569, 49-54	2.5	17
131	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, **2014**, 35, 611-21	3.5	17
130	Kohn's localization in the insulating state: one-dimensional lattices, crystalline versus disordered. *Journal of Chemical Physics*, **2010**, 133, 064703	3.9	17
129	Electron localizability and polarizability in tight-binding graphene nanostructures. *Theoretical Chemistry Accounts*, **2010**, 126, 257-263	1.9	17
128	End states and singlet triplet degeneracy in linear atomic chains. *Chemical Physics Letters*, **2008**, 465, 102-105	2.5	17
127	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. *Scientific Reports*, **2016**, 6, 28480	4.9	17
126	UV-vis absorption spectrum of a novel Ru(II) complex intercalated in DNA: [Ru(2,2'-bipy)(dppz)(2,2'-ArPy)]+. *Journal of Molecular Modeling*, **2014**, 20, 2082	2	16
125	DNA Photosensitization by an "Insider": Photophysics and Triplet Energy Transfer of 5-Methyl-2-pyrimidone Deoxyribonucleoside. *Chemistry - A European Journal*, **2015**, 21, 11509-16	4.8	16
124	Stability of the guanine endoperoxide intermediate: a computational challenge for density functional theory. *Journal of Physical Chemistry A*, **2014**, 118, 11612-9	2.8	15
123	Asymptotic analysis of the localization spread and polarizability of 1-D noninteracting electrons. *International Journal of Quantum Chemistry*, **2012**, 112, 653-664	2.1	15

122	Restoring the size consistency of multireference configuration interactions through class dressings: applications to ground and excited states. *Journal of Chemical Physics*, **2008**, 129, 064112	3.9	15
121	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions: A Test Study on the Neon Dimer. *Journal of Chemical Theory and Computation*, **2007**, 3, 477-85	6.4	15
120	A Davidson technique for the computation of dispersion constants: Full CI results for Be and LiH. *Chemical Physics*, **2004**, 306, 153-161	2.3	15
119	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. *Nucleic Acids Research*, **2017**, 45, 3654-3662	20.1	14
118	Exploring the Photophysics of Polyfluorinated Phthalocyanine Derivatives as Potential Theranostic Agents. *Journal of Physical Chemistry C*, **2019**, 123, 24417-24425	3.8	14
117	2,5-Dithienylpyrrole (DTP) as a donor component in DTPA organic sensitizers: photophysical and photovoltaic properties. *RSC Advances*, **2015**, 5, 4041-4050	3.7	14
116	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. *Physical Chemistry Chemical Physics*, **2017**, 19, 23187-23193	3.6	14
115	Photophysics of acetophenone interacting with DNA: why the road to photosensitization is open. *Photochemistry and Photobiology*, **2015**, 91, 323-30	3.6	14
114	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	14
113	Photophysical properties of bichromophoric Fe(II) complexes bearing an aromatic electron acceptor. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	13
112	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. *Frontiers in Chemistry*, **2018**, 6, 86	5	13
111	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. *Scientific Reports*, **2017**, 7, 8885	4.9	13
110	Full-configuration-interaction study of the metal-insulator transition in model systems: Peierls dimerization in H(n) rings and chains. *Journal of Chemical Physics*, **2013**, 138, 074315	3.9	13
109	A theoretical study of Be(N) linear chains: variational and perturbative approaches. *Journal of Chemical Physics*, **2009**, 131, 034309	3.9	13
108	Full configuration-interaction study of the metal-insulator transition in model systems. *Journal of Physics: Conference Series*, **2008**, 117, 012005	0.3	13
107	Fluorene-imidazole dyes excited states from first-principles calculations: topological insights. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
106	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
105	QM/MM calculation of absorption spectra of complex systems: The case of human serum albumin. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 360-366	2	12

104	Beryllium chains interacting with Graphene Nanoislands: From anti-ferromagnetic to ferromagnetic ground state. *Chemical Physics Letters*, **2010**, 496, 306-309	2.5	12
103	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3290-3296	6.4	11
102	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
101	Cooperative Effects of Cytosine Methylation on DNA Structure and Dynamics. *Journal of Physical Chemistry B*, **2019**, 123, 7365-7371	3.4	11
100	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
99	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. *Journal of Physical Chemistry Letters*, **2019**, 10, 6750-6754	6.4	11
98	Theoretical Study of BeN Linear Chains: Optimized Geometries and Harmonic Frequencies. *Journal of Chemical Theory and Computation*, **2009**, 5, 1266-73	6.4	11
97	Full Configuration-Interaction Study on the Tetrahedral Li4 Cluster. *Journal of Chemical Theory and Computation*, **2008**, 4, 404-13	6.4	11
96	Common Format for Quantum Chemistry Interoperability: Q5Cost Format and Library. *Lecture Notes in Computer Science*, **2008**, 1094-1107	0.9	11
95	Triplet photosensitization mechanism of thymine by an oxidized nucleobase: from a dimeric model to DNA environment. *Physical Chemistry Chemical Physics*, **2018**, 20, 25666-25675	3.6	11
94	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
93	Probing optical properties of thiophene derivatives for two-photon absorption. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	10
92	To what extent are the photophysical properties of quinoxaline- and quinoxalinone-based chromophores predictable?. *Dyes and Pigments*, **2019**, 170, 107580	4.6	10
91	Toward Luminescent Iron Complexes: Unravelling the Photophysics by Computing Potential Energy Surfaces. *ChemPhotoChem*, **2019**, 3, 666-683	3.3	10
90	Computational Modeling of Exciton Localization in Self-Assembled Perylene Helices: Effects of Thermal Motion and Aggregate Size. *Journal of Physical Chemistry C*, **2019**, 123, 6427-6437	3.8	10
89	Ionization and fragmentation of uracil upon microhydration. *Physical Chemistry Chemical Physics*, **2019**, 21, 4810-4821	3.6	10
88	Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates. *Chemical Communications*, **2020**, 56, 4404-4407	5.8	10
87	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

86	Molecular Bases of DNA Packaging in Bacteria Revealed by All-Atom Molecular Dynamics Simulations: The Case of Histone-Like Proteins in. *Journal of Physical Chemistry Letters*, **2019**, 10, 7200-7207	6.4	10
85	Determination of spin Hamiltonians from projected single reference configuration interaction calculations. I. Spin 1/2 systems. *Journal of Chemical Physics*, **2010**, 133, 044106	3.9	10
84	Probing halogen-halogen interactions in solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 32443-32450	3.6	9
83	Electronic bistability in linear beryllium chains. *Journal of Physical Chemistry A*, **2009**, 113, 5240-5	2.8	9
82	Make it clean, make it safe: A review on virus elimination via adsorption. *Chemical Engineering Journal*, **2021**, 412, 128682	14.7	9
81	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 33180-33186	3.6	9
80	Halochromic luminescent quinoxalinones as a basis for pH-sensing in organic and aqueous solutions. *Dyes and Pigments*, **2021**, 186, 108958	4.6	9
79	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. *Journal of Physical Chemistry Letters*, **2019**, 10, 7133-7140	6.4	8
78	Theoretical study of the excited state properties of luminescent phospholes. *Dyes and Pigments*, **2019**, 164, 363-371	4.6	8
77	The three Endonuclease III variants of Deinococcus radiodurans possess distinct and complementary DNA repair activities. *DNA Repair*, **2019**, 78, 45-59	4.3	8
76	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 4749-4757	3.6	8
75	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
74	Evaluation of temoporfin affinity to β-cyclodextrins assuming self-aggregation. *Journal of Photochemistry and Photobiology A: Chemistry*, **2018**, 367, 13-21	4.7	8
73	Targeting G-quadruplexes with Organic Dyes: Chelerythrine-DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. *Antioxidants*, **2019**, 8,	7.1	8
72	Coupled-Cluster study of lone-pair bonding in the tetrahedral Cu4 cluster. *Chemical Physics Letters*, **2011**, 503, 215-219	2.5	8
71	Photophysical Investigation of Iron(II) Complexes Bearing Bidentate Annulated Isomeric Pyridine-NHC Ligands. *Journal of Physical Chemistry C*, **2020**, 124, 18379-18389	3.8	8
70	drug discovery of IKK-β inhibitors from 2-amino-3-cyano-4-alkyl-6-(2-hydroxyphenyl) pyridine derivatives based on QSAR, docking, molecular dynamics and drug-likeness evaluation studies. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-17	3.6	8
69	Absorption Spectroscopy and Photophysics of a Re -dppz Probe for DNA-Mediated Charge Transport. *Chemistry - A European Journal*, **2018**, 24, 14425-14435	4.8	8

68	Triggering Tautomerization of Curcumin by Confinement into Liposomes. *ChemPhotoChem*, **2019**, 3, 1034-1041	3.3	7
67	Novel Ru-based sunlight harvesters bearing dithienylpyrrolo (DTP)-bipyridine ligands: Synthesis, characterization and photovoltaic properties. *Dyes and Pigments*, **2014**, 101, 318-328	4.6	7
66	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
65	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. *Physical Chemistry Chemical Physics*, **2020**, 22, 15496-15508	3.6	6
64	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
63	Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. *Frontiers in Chemistry*, **2015**, 3, 67	5	6
62	An enlarged basis Full-Cl calculation of C7 dispersion coefficients for the LiH□iH homodimer. *Chemical Physics Letters*, **2003**, 382, 393-398	2.5	6
61	Recent advances in iron-complexes as drug candidates for cancer therapy: reactivity, mechanism of action and metabolites. *Dalton Transactions*, **2020**, 49, 11451-11466	4.3	6
60	Probing interaction of a trilysine peptide with DNA underlying formation of guanine-lysine cross-links: insights from molecular dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 23418-23424	3.6	6
59	Human DNA Telomeres in Presence of Oxidative Lesions: The Crucial Role of Electrostatic Interactions on the Stability of Guanine Quadruplexes. *Antioxidants*, **2019**, 8,	7.1	5
58	Towards Iron(II) Complexes with Octahedral Geometry: Synthesis, Structure and Photophysical Properties. *Molecules*, **2020**, 25,	4.8	5
57	Blue satellites on He lines due to He-He collisions. *Astronomy and Astrophysics*, **2013**, 559, A70	5.1	5
56	Theoretical study of the absorption spectrum of a photoisomerizable iron complex. *Journal of Physical Chemistry A*, **2012**, 116, 11905-12	2.8	5
55	Heisenberg behavior of some carbon-beryllium compounds: How well truncated-CI approaches work. *Journal of Computational Chemistry*, **2011**, 32, 315-24	3.5	5
54	Mixed valence character of anionic linear beryllium chains: a CAS-SCF and MR-CI study. *Journal of Physical Chemistry A*, **2009**, 113, 14706-10	2.8	5
53	Frozen-core full-CI calculation of imaginary frequency-dependent dipole polarizabilities of ground state BeH2 and the C6 dispersion coefficients of its homodimer. *Chemical Physics Letters*, **2005**, 414, 51-54	2.5	5
52	Impact of the Nucleosome Histone Core on the Structure and Dynamics of DNA-Containing Pyrimidine-Pyrimidone (6-4) Photoproduct. *Journal of Chemical Theory and Computation*, **2020**, 16, 5972-5981	5.4	5
51	Photoisomerization of a biomimetic cyclocurcumin analogue rationalized by molecular modelling. *Physical Chemistry Chemical Physics*, **2021**, 23, 12842-12849	3.6	5

50	Large-Scale Quantum Monte Carlo Electronic Structure Calculations on the EGEE Grid **2012**, 195-207		5
49	The Non Empirical Local Self Consistent Field Method: Application to Quantum Mechanics/Molecular Mechanics (QM/MM) Modeling of Large Biomolecular Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 343-365	0.7	4
48	C-glyco"RGD" as □and □integrin ligands for imaging applications: Synthesis, in vitro evaluation and molecular modeling. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 4101-4109	3.4	4
47	Charge transfer and mixed-valence behavior in phtalocyanine-dimer cations. *Journal of Chemical Physics*, **2010**, 133, 124301	3.9	4
46	On the triplet ground state of tetrahedral X4 clusters (X = Li, Na, K, Cu). *Journal of Chemical Physics*, **2012**, 136, 094301	3.9	4
45	CI calculations of long-range C6 dispersion coefficients for BH□H. *Chemical Physics Letters*, **2008**, 450, 396-399	2.5	4
44	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
43	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
42	Experimental and theoretical studies on thymine photodimerization mediated by oxidatively generated DNA lesions and epigenetic intermediates. *Physical Chemistry Chemical Physics*, **2020**, 22, 25661-25668	3.6	4
41	Optical properties of photodynamic therapy drugs in different environments: the paradigmatic case of temoporfin. *Physical Chemistry Chemical Physics*, **2020**, 22, 16956-16964	3.6	4
40	Synthesis and Photoswitching Properties of Bioinspired Dissymmetric □Pyrone, an Analogue of Cyclocurcumin. *Journal of Organic Chemistry*, **2021**, 86, 8112-8126	4.2	4
39	Stimuli-responsive emission of quinoxalinone-based compounds. From experimental findings to theoretical insight by means of multiscale computational spectroscopy approaches. *Dyes and Pigments*, **2021**, 184, 108797	4.6	4
38	Photoinduced DNA Lesions in Dormant Bacteria: The Peculiar Route Leading to Spore Photoproducts Characterized by Multiscale Molecular Dynamics*. *Chemistry - A European Journal*, **2020**, 26, 14236-14241	4.8	3
37	Iron's Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. *Molecules*, **2020**, 25,	4.8	3
36	Ab Initio Study of the Stepwise versus Concerted Fragmentation Pathways in Microhydrated Thymine Radical Cations. *Chemistry - A European Journal*, **2019**, 25, 15525-15534	4.8	3
35	Insight on the interaction of polychlorobiphenyl with nucleic acid-base. *Journal of Molecular Modeling*, **2013**, 19, 581-8	2	3
34	Structure of the 5' untranslated region in SARS-CoV-2 genome and its specific recognition by innate immune system the human oligoadenylate synthase 1.. *Chemical Communications*, **2022**,	5.8	3
33	Conical intersection properties unraveled by the position spread tensor. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	3

32	The Electronic Structure of Graphene Nanoislands: A CAS-SCF and NEVPT2 Study. *Advances in Condensed Matter Physics*, **2018**, 2018, 1-14	1	3
31	2,3-(Dibenzimidazol-2-yl)quinoxalines: Unexpected Dynamical Effect on Steady-State Electronic Absorption Spectra. *Journal of Physical Chemistry B*, **2019**, 123, 5514-5523	3.4	2
30	DNA Nucleobase under Ionizing Radiation: Unexpected Proton Transfer by Thymine Cation in Water Nanodroplets. *Chemistry - A European Journal*, **2020**, 26, 11340-11344	4.8	2
29	Conformational changes of DNA induced by a trans-azobenzene derivative via non-covalent interactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 22645-22651	3.6	2
28	The Electronic Structure of Short Carbon Nanotubes: The Effects of Correlation. *Advances in Condensed Matter Physics*, **2015**, 2015, 1-14	1	2
27	Finite-Size Effects in Graphene Nanostructures **2011**,		2
26	High-spin states in tetrahedral X4 clusters (X = H, Li, Na, K). *International Journal of Quantum Chemistry*, **2009**, 110, NA-NA	2.1	2
25	Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure.. *Journal of Physical Chemistry A*, **2022**,	2.8	2
24	Don't help them to bury the light. The interplay between intersystem crossing and hydrogen transfer in photoexcited curcumin revealed by surface-hopping dynamics. *Physical Chemistry Chemical Physics*, **2021**, 23, 24757-24764	3.6	2
23	Quantum chemistry of the excited state: recent trends in methods developments and applications. *Photochemistry*, **2018**, 28-77	1.8	2
22	Forever Young: Structural Stability of Telomeric Guanine Quadruplexes in the Presence of Oxidative DNA Lesions*. *Chemistry - A European Journal*, **2021**, 27, 8865-8874	4.8	2
21	Staring at the Naked Goddess: Unraveling the Structure and Reactivity of Artemis Endonuclease Interacting with a DNA Double Strand. *Molecules*, **2021**, 26,	4.8	2
20	Triplet stabilization for enhanced drug photorelease from sunscreen-based photocages. *Organic and Biomolecular Chemistry*, **2021**, 19, 1752-1759	3.9	2
19	Recognition of a tandem lesion by DNA bacterial formamidopyrimidine glycosylases explored combining molecular dynamics and machine learning. *Computational and Structural Biotechnology Journal*, **2021**, 19, 2861-2869	6.8	2
18	A numerical method for computing dispersion constants. *Theoretical Chemistry Accounts*, **2009**, 123, 265-272	2.1	1
17	Comparative Study of Emission Spectra of He(3S)-He(2P) at 706 and 728 nm Due to the Triplet and Singlet Transitions. *Journal of Physics: Conference Series*, **2012**, 397, 012035	0.3	1
16	On the calculation of high-spin states in the full configuration-interaction formalism. *Chemical Physics*, **2008**, 348, 83-88	2.3	1
15	Structural and functional characterization of DdrC, a novel DNA damage-induced nucleoid associated protein involved in DNA compaction		1

14	Competition between the Photothermal Effect and Emission in Potential Phototherapy Agents. *Journal of Physical Chemistry B*, **2021**, 125, 8733-8741	3.4	1
13	Characterization of Conjugation Effects in the Series of Quinoxaline-2-ones by Means of Vibrational Raman Spectroscopy. *Journal of Physical Chemistry A*, **2020**, 124, 3865-3875	2.8	1
12	The Iron Maiden. Cytosolic Aconitase/IRP1 Conformational Transition in the Regulation of Ferritin Translation and Iron Hemostasis. *Biomolecules*, **2021**, 11,	5.9	1
11	DNA Photodamage and Repair: Computational Photobiology in Action. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 293-332	0.7	0
10	Bidentate pyridyl-NHC ligands: synthesis, ground and excited state properties of their iron(II) complexes and role of the fac/mer isomerism. *European Journal of Inorganic Chemistry*,	2.3	0
9	Origins of the photoinitiation capacity of aromatic thiols as photoinitiatiors: a computational study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24377-24385	3.6	0
8	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
7	Never Cared for What They Do: High Structural Stability of Guanine-Quadruplexes in the Presence of Strand-Break Damage. *Molecules*, **2022**, 27, 3256	4.8	0
6	Computational Study of Photo-oxidative Degradation Mechanisms of Boron-Containing Oligothiophenes. *Journal of Physical Chemistry A*, **2020**, 124, 1390-1398	2.8	
5	Towards an accurate treatment of □<-□transitions: Moving onto. *Chemical Physics Letters*, **2013**, 580, 14-20	2.5	
4	Hybrid QM/MM Methods: Treating Electronic Phenomena in Very Large Molecular Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2014**, 1-20	0.7	
3	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. *Highlights in Theoretical Chemistry*, **2014**, 39-47		
2	Nucleic Acids under Stress: Understanding and Simulating Nucleobase Fragmentation Pathways. *ChemPlusChem*, **2021**, 86, 1426-1435	2.8	
1	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	