Antonio Monari

List of Publications by Year in Descending Order

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	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
192	Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure.. *Journal of Physical Chemistry A*, **2022**,	2.8	2
191	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	
190	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
189	DNA Photodamage and Repair: Computational Photobiology in Action. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 293-332	0.7	0
188	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
187	Origins of the photoinitiation capacity of aromatic thiols as photoinitiators: a computational study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24377-24385	3.6	0
186	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
185	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
184	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
183	Make it clean, make it safe: A review on virus elimination via adsorption. *Chemical Engineering Journal*, **2021**, 412, 128682	14.7	9
182	Synthesis and Photoswitching Properties of Bioinspired Dissymmetric Pyrone, an Analogue of Cyclocurcumin. *Journal of Organic Chemistry*, **2021**, 86, 8112-8126	4.2	4
181	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
180	Competition between the Photothermal Effect and Emission in Potential Phototherapy Agents. *Journal of Physical Chemistry B*, **2021**, 125, 8733-8741	3.4	1
179	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
178	Triplet stabilization for enhanced drug photorelease from sunscreen-based photocages. *Organic and Biomolecular Chemistry*, **2021**, 19, 1752-1759	3.9	2
177	Halochromic luminescent quinoxalinones as a basis for pH-sensing in organic and aqueous solutions. *Dyes and Pigments*, **2021**, 186, 108958	4.6	9

176	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
175	Photoisomerization of a biomimetic cyclocurcumin analogue rationalized by molecular modelling. *Physical Chemistry Chemical Physics*, **2021**, 23, 12842-12849	3.6	5
174	The Iron Maiden. Cytosolic Aconitase/IRP1 Conformational Transition in the Regulation of Ferritin Translation and Iron Hemostasis. *Biomolecules*, **2021**, 11,	5.9	1
173	Nucleic Acids under Stress: Understanding and Simulating Nucleobase Fragmentation Pathways. *ChemPlusChem*, **2021**, 86, 1426-1435	2.8	
172	Towards Iron(II) Complexes with Octahedral Geometry: Synthesis, Structure and Photophysical Properties. *Molecules*, **2020**, 25,	4.8	5
171	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
170	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
169	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
168	Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates. *Chemical Communications*, **2020**, 56, 4404-4407	5.8	10
167	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
166	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
165	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. *Physical Chemistry Chemical Physics*, **2020**, 22, 15496-15508	3.6	6
164	Computational Study of Photo-oxidative Degradation Mechanisms of Boron-Containing Oligothiophenes. *Journal of Physical Chemistry A*, **2020**, 124, 1390-1398	2.8	
163	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 4749-4757	3.6	8
162	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
161	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
160	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
159	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

158	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
157	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
156	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
155	drug discovery of IKK-□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
154	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
153	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
152	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. *Journal of Physical Chemistry Letters*, **2019**, 10, 7133-7140	6.4	8
151	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
150	Exploring the Photophysics of Polyfluorinated Phthalocyanine Derivatives as Potential Theranostic Agents. *Journal of Physical Chemistry C*, **2019**, 123, 24417-24425	3.8	14
149	Theoretical study of the excited state properties of luminescent phospholes. *Dyes and Pigments*, **2019**, 164, 363-371	4.6	8
148	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
147	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
146	Photophysical properties of bichromophoric Fe(II) complexes bearing an aromatic electron acceptor. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	13
145	To what extent are the photophysical properties of quinoxaline- and quinoxalinone-based chromophores predictable?. *Dyes and Pigments*, **2019**, 170, 107580	4.6	10
144	Triggering Tautomerization of Curcumin by Confinement into Liposomes. *ChemPhotoChem*, **2019**, 3, 1034-1041	3.3	17
143	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
142	Toward Luminescent Iron Complexes: Unravelling the Photophysics by Computing Potential Energy Surfaces. *ChemPhotoChem*, **2019**, 3, 666-683	3.3	10
141	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

140	The three Endonuclease III variants of Deinococcus radiodurans possess distinct and complementary DNA repair activities. *DNA Repair*, **2019**, 78, 45-59	4.3	8
139	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
138	Ionization and fragmentation of uracil upon microhydration. *Physical Chemistry Chemical Physics*, **2019**, 21, 4810-4821	3.6	10
137	Cooperative Effects of Cytosine Methylation on DNA Structure and Dynamics. *Journal of Physical Chemistry B*, **2019**, 123, 7365-7371	3.4	11
136	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
135	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
134	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
133	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. *Journal of Physical Chemistry Letters*, **2019**, 10, 6750-6754	6.4	11
132	Targeting G-quadruplexes with Organic Dyes: Chelerythrine-DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. *Antioxidants*, **2019**, 8,	7.1	8
131	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
130	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
129	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
128	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
127	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
126	NHC-Based Iron Sensitizers for DSSCs. *Inorganics*, **2018**, 6, 63	2.9	55
125	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
124	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. *Frontiers in Chemistry*, **2018**, 6, 86	5	13
123	Evaluation of temoporfin affinity to □cyclodextrins assuming self-aggregation. *Journal of Photochemistry and Photobiology A: Chemistry*, **2018**, 367, 13-21	4.7	8

122	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
121	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
120	Quantum chemistry of the excited state: recent trends in methods developments and applications. *Photochemistry*, **2018**, 28-77	1.8	2
119	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
118	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
117	Conical intersection properties unraveled by the position spread tensor. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	3
116	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. *Frontiers in Chemistry*, **2018**, 6, 495	5	21
115	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
114	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. *Molecules*, **2018**, 23,	4.8	49
113	The Electronic Structure of Graphene Nanoislands: A CAS-SCF and NEVPT2 Study. *Advances in Condensed Matter Physics*, **2018**, 2018, 1-14	1	3
112	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
111	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
110	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. *RSC Advances*, **2017**, 7, 10992-10999	3.7	27
109	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. *Nucleic Acids Research*, **2017**, 45, 3654-3662	20.1	14
108	Probing optical properties of thiophene derivatives for two-photon absorption. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	10
107	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3290-3296	6.4	11
106	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
105	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

104	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
103	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. *Scientific Reports*, **2017**, 7, 8885	4.9	13
102	Molecular Dynamics Insights into Polyamine-DNA Binding Modes: Implications for Cross-Link Selectivity. *Chemistry - A European Journal*, **2017**, 23, 12845-12852	4.8	21
101	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
100	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. *Physical Chemistry Chemical Physics*, **2017**, 19, 23187-23193	3.6	14
99	Probing halogen-halogen interactions in solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 32443-32450	3.6	9
98	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. *Journal of Physical Chemistry C*, **2016**, 120, 17916-17926	3.8	28
97	Interfacial charge separation and photovoltaic efficiency in Fe(ii)-carbene sensitized solar cells. *Physical Chemistry Chemical Physics*, **2016**, 18, 28069-28081	3.6	41
96	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
95	Probing the reactivity of singlet oxygen with purines. *Nucleic Acids Research*, **2016**, 44, 56-62	20.1	44
94	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. *Physical Chemistry Chemical Physics*, **2016**, 18, 7829-36	3.6	22
93	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
92	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
91	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
90	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. *Scientific Reports*, **2016**, 6, 28480	4.9	17
89	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 33180-33186	3.6	9
88	Fluorene-imidazole dyes excited states from first-principles calculations□topological insights. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
87	A new record excited state (3)MLCT lifetime for metalorganic iron(ii) complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 12550-6	3.6	99

86	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
85	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
84	Modeling DNA electronic circular dichroism by QM/MM methods and Frenkel Hamiltonian. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	19
83	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
82	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
81	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
80	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
79	Understanding DNA under oxidative stress and sensitization: the role of molecular modeling. *Frontiers in Chemistry*, **2015**, 3, 43	5	42
78	Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. *Frontiers in Chemistry*, **2015**, 3, 67	5	6
77	The Electronic Structure of Short Carbon Nanotubes: The Effects of Correlation. *Advances in Condensed Matter Physics*, **2015**, 2015, 1-14	1	2
76	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. *Journal of Physical Chemistry Letters*, **2015**, 6, 576-80	6.4	40
75	Photophysics of acetophenone interacting with DNA: why the road to photosensitization is open. *Photochemistry and Photobiology*, **2015**, 91, 323-30	3.6	14
74	Interaction of palmatine with DNA: an environmentally controlled phototherapy drug. *Journal of Physical Chemistry B*, **2015**, 119, 410-9	3.4	36
73	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
72	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
71	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
70	All-organic chromophores for dye-sensitized solar cells: A theoretical study on aggregation. *Dyes and Pigments*, **2014**, 101, 203-211	4.6	21
69	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

68	Toward a Quantitative Assessment of Electronic Transitions' Charge-Transfer Character. *Journal of Chemical Theory and Computation*, **2014**, 10, 3896-905	6.4	114
67	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
66	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
65	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
64	Lipid Peroxidation in Membranes: The Peroxyl Radical Does Not "Float". *Journal of Physical Chemistry Letters*, **2014**, 5, 1653-8	6.4	55
63	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
62	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	
61	Heteroleptic Pyridyl-Carbene Iron Complexes with Tuneable Electronic Properties. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3747-3753	2.3	52
60	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
59	Theoretical computation of Betain B30 solvatochromism using a Polarizable Continuum Model. *Dyes and Pigments*, **2014**, 100, 24-31	4.6	29
58	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. *Highlights in Theoretical Chemistry*, **2014**, 39-47		
57	A FCI benchmark on beryllium dimer: The lowest singlet and triplet states. *Chemical Physics Letters*, **2013**, 568-569, 49-54	2.5	17
56	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
55	Insight on the interaction of polychlorobiphenyl with nucleic acid-base. *Journal of Molecular Modeling*, **2013**, 19, 581-8	2	3
54	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
53	Towards an accurate treatment of □<-□transitions: Moving onto. *Chemical Physics Letters*, **2013**, 580, 14-20	2.5	
52	Blue satellites on He lines due to He-He collisions. *Astronomy and Astrophysics*, **2013**, 559, A70	5.1	5
51	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

50	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
49	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
48	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
47	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
46	Theoretical study of the absorption spectrum of a photoisomerizable iron complex. *Journal of Physical Chemistry A*, **2012**, 116, 11905-12	2.8	5
45	A QM/MM study on the spinach plastocyanin: Redox properties and absorption spectra. *Computational and Theoretical Chemistry*, **2012**, 990, 119-125	2	54
44	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
43	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
42	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
41	Strong π-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
40	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	14
39	A priori modeling of chemical reactions on computational grid platforms: Workflows and data models. *Chemical Physics*, **2012**, 398, 192-198	2.3	23
38	On the triplet ground state of tetrahedral X4 clusters (X = Li, Na, K, Cu). *Journal of Chemical Physics*, **2012**, 136, 094301	3.9	4
37	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
36	Large-Scale Quantum Monte Carlo Electronic Structure Calculations on the EGEE Grid **2012**, 195-207		5
35	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
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