Roberto Improta

List of Publications by Year in Descending Order

211 papers	9,837 citations	51 h-index	91 g-index
227 ext. papers	10,649 ext. citations	6.1 avg, IF	6.43 L-index

#	Paper	IF	Citations
211	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
210	Early steps of oxidative damage in DNA quadruplexes are position-dependent: Quantum mechanical and molecular dynamics analysis of human telomeric sequence containing ionized guanine. *International Journal of Biological Macromolecules*, **2021**, 194, 882-882	7.9	1
209	The Ultrafast Quantum Dynamics of Photoexcited Adenine-Thymine Basepair Investigated with a Fragment-based Diabatization and a Linear Vibronic Coupling Model. *Journal of Physical Chemistry A*, **2021**, 125, 8912-8924	2.8	1
208	Excitonic Model for Strongly Coupled Multichromophoric Systems: The Electronic Circular Dichroism Spectra of Guanine Quadruplexes as Test Cases. *Journal of Chemical Theory and Computation*, **2021**, 17, 405-415	6.4	9
207	Nonadiabatic Absorption Spectra and Ultrafast Dynamics of DNA and RNA Photoexcited Nucleobases. *Molecules*, **2021**, 26,	4.8	8
206	Solvent-Dependent Stabilization of a Charge Transfer State is the Key to Ultrafast Triplet State Formation in an Epigenetic DNA Nucleoside. *Chemistry - A European Journal*, **2021**, 27, 10932-10940	4.8	3
205	Fragment Diabatization Linear Vibronic Coupling Model for Quantum Dynamics of Multichromophoric Systems: Population of the Charge-Transfer State in the Photoexcited Guanine-Cytosine Pair. *Journal of Chemical Theory and Computation*, **2021**, 17, 4660-4674	6.4	8
204	Excited-State Absorption of Uracil in the Gas Phase: Mapping the Main Decay Paths by Different Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2021**, 17, 1638-1652	6.4	6
203	Adenine Radical Cation Formation by a Ligand-Centered Excited State of an Intercalated Chromium Polypyridyl Complex Leads to Enhanced DNA Photo-oxidation. *Journal of the American Chemical Society*, **2021**, 143, 14766-14779	16.4	6
202	The Structural Duality of Nucleobases in Guanine Quadruplexes Controls Their Low-Energy Photoionization. *Journal of Physical Chemistry Letters*, **2021**, 12, 8309-8313	6.4	0
201	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. *Physical Chemistry Chemical Physics*, **2021**, 23, 8181-8199	3.6	7
200	The Excited State Dynamics of a Mutagenic Cytidine Etheno Adduct Investigated by Combining Time-Resolved Spectroscopy and Quantum Mechanical Calculations.. *Journal of Physical Chemistry Letters*, **2021**, 251-257	6.4	0
199	Deciphering the pH-dependence of ground- and excited-state equilibria of thienoguanine. *Physical Chemistry Chemical Physics*, **2020**, 22, 7381-7391	3.6	5
198	Excited State Dynamics of 8-Vinyldeoxyguanosine In Aqueous Solution Studied by Time-Resolved Fluorescence Spectroscopy and Quantum Mechanical Calculations. *Molecules*, **2020**, 25,	4.8	2
197	Potassium Ions Enhance Guanine Radical Generation upon Absorption of Low-Energy Photons by G-Quadruplexes and Modify Their Reactivity. *Journal of Physical Chemistry Letters*, **2020**, 11, 1305-1309	6.4	10
196	Vibrations of the guanine-cytosine pair in chloroform: an anharmonic computational study. *Physical Chemistry Chemical Physics*, **2020**, 22, 5509-5522	3.6	1
195	Quantum dynamics of the π/nπ decay of the epigenetic nucleobase 1,5-dimethyl-cytosine in the gas phase. *Physical Chemistry Chemical Physics*, **2020**, 22, 26525-26535	3.6	4

194	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. *Journal of Chemical Theory and Computation*, **2020**, 16, 1215-1231	6.4	23
193	Ultrafast Dynamics of the Two Lowest Bright Excited States of Cytosine and 1-Methylcytosine: A Quantum Dynamical Study. *Journal of Chemical Theory and Computation*, **2020**, 16, 5792-5808	6.4	17
192	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. *Journal of Chemical Theory and Computation*, **2020**, 16, 7061-7077	6.4	7
191	What Makes Thienoguanosine an Outstanding Fluorescent DNA Probe?. *Journal of the American Chemical Society*, **2020**, 142, 16999-17014	16.4	9
190	Studying the excited electronic states of guanine rich DNA quadruplexes by quantum mechanical methods: main achievements and perspectives. *Photochemical and Photobiological Sciences*, **2020**, 19, 436-444	4.2	10
189	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. *ChemPhotoChem*, **2019**, 3, 846-855	3.3	6
188	Radicals Generated in Tetramolecular Guanine Quadruplexes by Photoionization: Spectral and Dynamical Features. *Journal of Physical Chemistry B*, **2019**, 123, 4950-4957	3.4	14
187	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 2885-2891	6.4	8
186	Excited-State Dynamics of Thienoguanosine, an Isomorphic Highly Fluorescent Analogue of Guanosine. *Chemistry - A European Journal*, **2019**, 25, 7375-7386	4.8	5
185	Unveiling Excited-State Chirality of Binaphthols by Femtosecond Circular Dichroism and Quantum Chemical Calculations. *Journal of Physical Chemistry Letters*, **2019**, 10, 4089-4094	6.4	14
184	Comprehensive Study of Guanine Excited State Relaxation and Photoreactivity in G-quadruplexes. *Journal of Physical Chemistry Letters*, **2019**, 10, 6873-6877	6.4	18
183	A multi-scale time-resolved study of photoactivated dynamics in 5-benzyl uracil, a model for DNA/protein interactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 26301-26310	3.6	4
182	The optical properties of adenine cation in different oligonucleotides: a PCM/TD-DFT study. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	1
181	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the (pi pi ^*/npi ^*) decay of thymine. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
180	Light induced damage and repair in nucleic acids and proteins: general discussion. *Faraday Discussions*, **2018**, 207, 389-408	3.6	
179	Toward a general mixed quantum/classical method for the calculation of the vibronic ECD of a flexible dye molecule with different stable conformers: Revisiting the case of 2,2,2-trifluoro-anthrylethanol. *Chirality*, **2018**, 30, 730-743	2.1	7
178	Photocrosslinking between nucleic acids and proteins: general discussion. *Faraday Discussions*, **2018** , 207, 283-306	3.6	5
177	Bionanophotonics: general discussion. *Faraday Discussions*, **2018**, 207, 491-512	3.6	

176	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. *Physical Chemistry Chemical Physics*, **2018**, 20, 6877-6890	3.6	32
175	Sequence dependence on DNA photochemistry: a computational study of photodimerization pathways in TpdC and dCpT dinucleotides. *Photochemical and Photobiological Sciences*, **2018**, 17, 586-591	4.2	5
174	Photoactivated proton coupled electron transfer in DNA: insights from quantum mechanical calculations. *Faraday Discussions*, **2018**, 207, 199-216	3.6	12
173	Adenine radicals generated in alternating AT duplexes by direct absorption of low-energy UV radiation. *Faraday Discussions*, **2018**, 207, 181-197	3.6	23
172	Radicals generated in alternating guanine-cytosine duplexes by direct absorption of low-energy UV radiation. *Physical Chemistry Chemical Physics*, **2018**, 20, 21381-21389	3.6	12
171	Topology Controls the Electronic Absorption and Delocalization of Electron Holes in Guanine Quadruplexes. *Chemistry - A European Journal*, **2018**, 24, 15185-15189	4.8	15
170	Development and Validation of Quantum Mechanically Derived Force-Fields: Thermodynamic, Structural, and Vibrational Properties of Aromatic Heterocycles. *Journal of Chemical Theory and Computation*, **2018**, 14, 4884-4900	6.4	16
169	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. *Chemical Physics*, **2018**, 515, 493-501	2.3	2
168	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. *Chemical Physics*, **2018**, 515, 452-463	2.3	15
167	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The π/π* Decay of Thymine in Water as a Test Case. *Journal of Chemical Theory and Computation* , **2018**, 14, 820-832	6.4	20
166	Photophysics of Deoxycytidine and 5-Methyldeoxycytidine in Solution: A Comprehensive Picture by Quantum Mechanical Calculations and Femtosecond Fluorescence Spectroscopy. *Journal of the American Chemical Society*, **2017**, 139, 7780-7791	16.4	49
165	Novel adenine/thymine photodimerization channels mapped by PCM/TD-DFT calculations on dApT and TpdA dinucleotides. *Photochemical and Photobiological Sciences*, **2017**, 16, 1277-1283	4.2	7
164	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. *Journal of Physical Chemistry Letters*, **2017**, 8, 1777-1783	6.4	43
163	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. *Journal of Chemical Theory and Computation*, **2017**, 13, 4636-4648	6.4	41
162	Absorption of Low-Energy UV Radiation by Human Telomere G-Quadruplexes Generates Long-Lived Guanine Radical Cations. *Journal of the American Chemical Society*, **2017**, 139, 10561-10568	16.4	44
161	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. *Photochemical and Photobiological Sciences*, **2017**, 16, 1415-1423	4.2	10
160	Multiple Electronic and Structural Factors Control Cyclobutane Pyrimidine Dimer and 6-4 Thymine-Thymine Photodimerization in a DNA Duplex. *Chemistry - A European Journal*, **2017**, 23, 15177-15188	4.8	32
159	Specific Recognition of G-Quadruplexes Over Duplex-DNA by a Macromolecular NIR Two-Photon Fluorescent Probe. *Journal of Physical Chemistry Letters*, **2017**, 8, 5915-5920	6.4	18

158	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine–Cytosine stacked dimer in water solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
157	Computing the Absorption and Emission Spectra of 5-Methylcytidine in Different Solvents: A Test-Case for Different Solvation Models. *Journal of Chemical Theory and Computation*, **2016**, 12, 4430-9	6.4	30
156	UV-Induced Adenine Radicals Induced in DNA A-Tracts: Spectral and Dynamical Characterization. *Journal of Physical Chemistry Letters*, **2016**, 7, 3949-3953	6.4	29
155	Photoinduced long-lived charge transfer excited states in AT-DNA strands. *Physical Chemistry Chemical Physics*, **2016**, 18, 21241-5	3.6	23
154	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
153	High-Energy Long-Lived Mixed Frenkel-Charge-Transfer Excitons: From Double Stranded (AT)n to Natural DNA. *Chemistry - A European Journal*, **2016**, 22, 4904-14	4.8	16
152	The absorption and emission spectra in solution of oligothiophene-based push–pull biomarkers: a PCM/TD-DFT vibronic study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
151	Predicting light absorption properties of anthocyanidins in solution: a multi-level computational approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
150	Excited-State Dynamics of DNA Duplexes with Different H-Bonding Motifs. *Journal of Physical Chemistry Letters*, **2016**, 7, 950-4	6.4	30
149	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. *Chemical Reviews*, **2016**, 116, 3540-93	68.1	291
148	Tautomers of a Fluorescent G Surrogate and Their Distinct Photophysics Provide Additional Information Channels. *Angewandte Chemie - International Edition*, **2016**, 55, 7974-7978	16.4	29
147	Tautomers of a Fluorescent G Surrogate and Their Distinct Photophysics Provide Additional Information Channels. *Angewandte Chemie*, **2016**, 128, 8106-8110	3.6	9
146	Effect of C5-Methylation of Cytosine on the UV-Induced Reactivity of Duplex DNA: Conformational and Electronic Factors. *Journal of Physical Chemistry B*, **2016**, 120, 4232-42	3.4	24
145	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	18
144	Excited State Pathways Leading to Formation of Adenine Dimers. *Journal of Physical Chemistry Letters*, **2016**, 7, 2020-3	6.4	18
143	A State-Specific PCM–DFT method to include dynamic solvent effects in the calculation of ionization energies: Application to DNA bases. *Chemical Physics Letters*, **2015**, 634, 20-24	2.5	14
142	Intramolecular vibrational redistribution in the non-radiative excited state decay of uracil in the gas phase: an ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2015**, 17, 11615-26	3.6	7
141	Absorption and emission spectral shapes of a prototype dye in water by combining classical/dynamical and quantum/static approaches. *Journal of Physical Chemistry A*, **2015**, 119, 5426-38	2.8	45

140	BALOO: A Fast and Versatile Code for Accurate Multireference Variational/Perturbative Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2024-35	6.4	10
139	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 5810-25	6.4	54
138	On the trade-off between processability and opto-electronic properties of single wall carbon nanotube derivatives in thin film heterojunctions. *Journal of Materials Chemistry C*, **2015**, 3, 303-312	7.1	18
137	The determinants of bond angle variability in protein/peptide backbones: A comprehensive statistical/quantum mechanics analysis. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1973-86	4.2	6
136	Bond distances in polypeptide backbones depend on the local conformation. *Acta Crystallographica Section D: Biological Crystallography*, **2015**, 71, 1272-83		8
135	UV-Induced Proton Transfer between DNA Strands. *Journal of the American Chemical Society*, **2015**, 137, 7059-62	16.4	103
134	Ultrafast Excited-State Deactivation of 8-Hydroxy-2'-deoxyguanosine Studied by Femtosecond Fluorescence Spectroscopy and Quantum-Chemical Calculations. *Journal of Physical Chemistry A*, **2015**, 119, 6131-9	2.8	13
133	Stabilization of Mixed Frenkel-Charge Transfer Excitons Extended Across Both Strands of Guanine-Cytosine DNA Duplexes. *Journal of Physical Chemistry Letters*, **2015**, 6, 2247-51	6.4	27
132	Photoinduced Electron Transfer in DNA: Charge Shift Dynamics Between 8-Oxo-Guanine Anion and Adenine. *Journal of Physical Chemistry B*, **2015**, 119, 7491-502	3.4	25
131	Perturbative multireference configuration interaction (CI-MRPT2) calculations in a focused dynamical approach: a computational study of solvatochromism in pyrimidine. *Journal of Physical Chemistry A*, **2015**, 119, 5250-9	2.8	9
130	TD-DFT investigation of the magnetic circular dichroism spectra of some purine and pyrimidine bases of nucleic acids. *Journal of Physical Chemistry A*, **2015**, 119, 5476-89	2.8	18
129	Excited states behavior of nucleobases in solution: insights from computational studies. *Topics in Current Chemistry*, **2015**, 355, 329-57		36
128	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 328-337	2	77
127	The excited state behavior of cytosine in the gas phase: A TD-DFT study. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 186-194	2	24
126	Mode-specific vibrational relaxation of photoexcited guanosine 5'-monophosphate and its acid form: a femtosecond broadband mid-IR transient absorption and theoretical study. *Physical Chemistry Chemical Physics*, **2014**, 16, 1487-99	3.6	22
125	Relative Stability of the La and Lb Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. *Journal of Physical Chemistry Letters*, **2014**, 5, 1806-11	6.4	34
124	Effect of C5-methylation of cytosine on the photoreactivity of DNA: a joint experimental and computational study of TCG trinucleotides. *Journal of the American Chemical Society*, **2014**, 136, 10838-41	16.4	46
123	Quantum-classical calculation of the absorption and emission spectral shapes of oligothiophenes at low and room temperature by first-principle calculations. *ChemPhysChem*, **2014**, 15, 3320-33	3.2	22

122	Quantum mechanical calculations unveil the structure and properties of the absorbing and emitting excited electronic states of guanine quadruplex. *Chemistry - A European Journal*, **2014**, 20, 8106-15	4.8	29
121	Efficient UV-induced charge separation and recombination in an 8-oxoguanine-containing dinucleotide. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 11612-7	11.5	57
120	The interplay between neutral exciton and charge transfer states in single-strand polyadenine: a quantum dynamical investigation. *Photochemical and Photobiological Sciences*, **2013**, 12, 1527-43	4.2	16
119	A joint experimental/theoretical study of the ultrafast excited state deactivation of deoxyadenosine and 9-methyladenine in water and acetonitrile. *Photochemical and Photobiological Sciences*, **2013**, 12, 1375-86	4.2	34
118	Absorption and Emission Spectra of a Flexible Dye in Solution: a Computational Time-Dependent Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4507-4516	6.4	66
117	Quantum-classical effective-modes dynamics of the pipi* --> npi* decay in 9H-adenine. A quadratic vibronic coupling model. *Faraday Discussions*, **2013**, 163, 223-42; discussion 243-75	3.6	38
116	Computational design, synthesis, and mechanochromic properties of new thiophene-based π-conjugated chromophores. *Chemistry - A European Journal*, **2013**, 19, 1996-2004	4.8	41
115	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. *Journal of Chemical Theory and Computation*, **2013**, 9, 2072-82	6.4	166
114	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. *Physical Chemistry Chemical Physics*, **2013**, 15, 3736-51	3.6	69
113	UV-light-induced hydrogen transfer in guanosine-guanosine aggregates. *Chemistry - A European Journal*, **2013**, 19, 5425-31	4.8	11
112	Multi-pathway excited state relaxation of adenine oligomers in aqueous solution: a joint theoretical and experimental study. *Chemistry - A European Journal*, **2013**, 19, 3762-74	4.8	53
111	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. *Highlights in Theoretical Chemistry*, **2013**, 339-350		
110	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Highlights in Theoretical Chemistry*, **2013**, 319-337		
109	The effect of methylation on the excited state dynamics of aminouracils. *Journal of Photochemistry and Photobiology A: Chemistry*, **2012**, 234, 37-43	4.7	5
108	Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 4483-93	6.4	58
107	Barrierless photoisomerisation of the "simplest cyanine": joining computational and femtosecond optical spectroscopies to trace the full reaction path. *Physical Chemistry Chemical Physics*, **2012**, 14, 13350-64	3.6	28
106	Photophysics and photochemistry of thymine deoxy-dinucleotide in water: a PCM/TD-DFT quantum mechanical study. *Journal of Physical Chemistry B*, **2012**, 116, 14261-74	3.4	50
105	Electronic excited states responsible for dimer formation upon UV absorption directly by thymine strands: joint experimental and theoretical study. *Journal of the American Chemical Society*, **2012**, 134, 14834-45	16.4	115

104	Cation Effect on the Electronic Excited States of Guanine Nanostructures Studied by Time-Resolved Fluorescence Spectroscopy. *Journal of Physical Chemistry C*, **2012**, 116, 14682-14689	3.8	39
103	Solvent effects on electron-driven proton-transfer processes: adenine-thymine base pairs. *Physical Chemistry Chemical Physics*, **2012**, 14, 8981-9	3.6	51
102	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	63
101	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	5
100	Excited state proton transfer is not involved in the ultrafast deactivation of Guanine-Cytosine pair in solution. *Journal of the American Chemical Society*, **2011**, 133, 19664-7	16.4	51
99	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 17007-12	3.6	81
98	Femtosecond fluorescence studies of DNA/RNA constituents. *Journal of Physics: Conference Series*, **2011**, 261, 012009	0.3	7
97	The interplay between π/nπ excited states in gas-phase thymine: a quantum dynamical study. *ChemPhysChem*, **2011**, 12, 1957-68	3.2	39
96	Interplay between Neutral and Charge-Transfer Excimers Rules the Excited State Decay in Adenine-Rich Polynucleotides. *Angewandte Chemie*, **2011**, 123, 12222-12225	3.6	13
95	Interplay between "neutral" and "charge-transfer" excimers rules the excited state decay in adenine-rich polynucleotides. *Angewandte Chemie - International Edition*, **2011**, 50, 12016-9	16.4	66
94	UV Visible Absorption and Emission Energies in Condensed Phase by PCM/TD-DFT Methods **2011**, 37-75		7
93	Peptide bond distortions from planarity: new insights from quantum mechanical calculations and peptide/protein crystal structures. *PLoS ONE*, **2011**, 6, e24533	3.7	35
92	DNA/RNA: Building Blocks of Life Under UV Irradiation. *Journal of Physical Chemistry Letters*, **2010**, 1, 2025-2030	6.4	159
91	Optical Properties of Guanine Nanowires: Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2010**, 114, 14339-14346	3.8	34
90	The peculiar spectral properties of amino-substituted uracils: a combined theoretical and experimental study. *Journal of Physical Chemistry B*, **2010**, 114, 12708-19	3.4	19
89	The excited electronic states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study. *Physical Chemistry Chemical Physics*, **2010**, 12, 4934-48	3.6	43
88	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. *Physical Chemistry Chemical Physics*, **2010**, 12, 10550-61	3.6	41
87	Time-dependent and time-independent approaches for the computation of absorption spectra of Uracil derivatives in solution. *International Journal of Quantum Chemistry*, **2010**, 110, 624-636	2.1	12

86	Three-dimensional diabatic models for the π -> nπ excited-state decay of uracil derivatives in solution. *Theoretical Chemistry Accounts*, **2009**, 123, 273-286	1.9	16
85	Role of side chains in collagen triple helix stabilization and partner recognition. *Journal of Peptide Science*, **2009**, 15, 131-40	2.1	38
84	PCM/TD-DFT study of the two lowest excited states of uracil derivatives in solution: The effect of the functional and of the cavity model. *Computational and Theoretical Chemistry*, **2009**, 914, 87-93		31
83	Photoinduced dynamics of guanosine monophosphate in water from broad-band transient absorption spectroscopy and quantum-chemical calculations. *Journal of the American Chemical Society*, **2009**, 131, 5839-50	16.4	90
82	Quantum dynamics of the ultrafast pi pi*/n pi* population transfer in uracil and 5-fluoro-uracil in water and acetonitrile. *Journal of Physical Chemistry B*, **2009**, 113, 14491-503	3.4	58
81	The polarizability in solution of tetra-phenyl-porphyrin derivatives in their excited electronic states: a PCM/TD-DFT study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4664-73	3.6	56
80	Excited states decay of the A-T DNA: A PCM/TD-DFT study in aqueous solution of the (9-methyl-adenine)(2).(1-methyl-thymine)(2) stacked tetramer. *Journal of the American Chemical Society*, **2009**, 131, 15232-45	16.4	99
79	On the controversial nature of the 1 1B(u) and 2 1B(u) states of trans-stilbene: the n-electron valence state perturbation theory approach. *Journal of Chemical Physics*, **2009**, 130, 174307	3.9	25
78	Vibronic model for the quantum dynamical study of the competition between bright and charge-transfer excited states in single-strand polynucleotides: the adenine dimer case. *Journal of Physical Chemistry A*, **2009**, 113, 15346-54	2.8	54
77	Quantum mechanical computations and spectroscopy: from small rigid molecules in the gas phase to large flexible molecules in solution. *Accounts of Chemical Research*, **2008**, 41, 605-16	24.3	142
76	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect: the Qx band of porphyrin as a case study. *Journal of Chemical Physics*, **2008**, 128, 224311	3.9	418
75	Effect of amino substitution on the excited state dynamics of uracil. *Photochemical and Photobiological Sciences*, **2008**, 7, 765-8	4.2	17
74	The decay from the dark npi* excited state in uracil: an integrated CASPT2/CASSCF and PCM/TD-DFT study in the gas phase and in water. *Journal of Physical Chemistry B*, **2008**, 112, 10769-72	3.4	61
73	The excited states of adenine and thymine nucleoside and nucleotide in aqueous solution: a comparative study by time-dependent DFT calculations. *Theoretical Chemistry Accounts*, **2008**, 120, 491-497	1.9	45
72	Absorption spectrum of A-T DNA unraveled by quantum mechanical calculations in solution on the (dA)2 x (dT)2 tetramer. *ChemPhysChem*, **2008**, 9, 2531-7	3.2	36
71	Can TD-DFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. *Journal of Computational Chemistry*, **2008**, 29, 957-64	3.5	56
70	Assessing solvent effects on the singlet excited state lifetime of uracil derivatives: A femtosecond fluorescence upconversion study in alcohols and D2O. *Chemical Physics*, **2008**, 350, 186-192	2.3	35
69	Contribution of dipole-dipole interactions to the stability of the collagen triple helix. *Protein Science*, **2008**, 17, 955-61	6.3	29

68	The excited states of pi-stacked 9-methyladenine oligomers: a TD-DFT study in aqueous solution. *Physical Chemistry Chemical Physics*, **2008**, 10, 2656-64	3.6	75
67	Accurate steady-state and zero-time fluorescence spectra of large molecules in solution by a first-principle computational method. *Journal of Physical Chemistry B*, **2007**, 111, 14080-2	3.4	53
66	Ab initio calculations of absorption spectra of large molecules in solution: coumarin C153. *Angewandte Chemie - International Edition*, **2007**, 46, 405-8	16.4	157
65	Solvent effects on the steady-state absorption and fluorescence spectra of uracil, thymine and 5-fluorouracil. *Photochemistry and Photobiology*, **2007**, 83, 595-9	3.6	37
64	Excited state properties of sizable molecules in solution: from structure to reactivity. *Theoretical Chemistry Accounts*, **2007**, 117, 1073-1084	1.9	9
63	UV-vis spectra of p-benzoquinone anion radical in solution by a TD-DFT/PCM approach. *Theoretical Chemistry Accounts*, **2007**, 118, 143-148	1.9	6
62	Influence of base stacking on excited-state behavior of polyadenine in water, based on time-dependent density functional calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 9931-6	11.5	119
61	Towards the Understanding of the Excited State Dynamics of Nucleic Acids: Solvent and Stacking Effect on the Photophysical Behavior of Nucleobases. *AIP Conference Proceedings*, **2007**,	0	2
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