Roberto Improta

List of Publications by Citations

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	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. *Journal of Chemical Physics*, **2006**, 125, 054103	3.9	586
210	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
209	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. *Journal of Chemical Physics*, **2007**, 126, 084509	3.9	398
208	Toward effective and reliable fluorescence energies in solution by a new state specific polarizable continuum model time dependent density functional theory approach. *Journal of Chemical Physics*, **2007**, 127, 074504	3.9	384
207	Singlet excited-state behavior of uracil and thymine in aqueous solution: a combined experimental and computational study of 11 uracil derivatives. *Journal of the American Chemical Society*, **2006**, 128, 607-19	16.4	336
206	Interplay of electronic, environmental, and vibrational effects in determining the hyperfine coupling constants of organic free radicals. *Chemical Reviews*, **2004**, 104, 1231-54	68.1	298
205	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. *Chemical Reviews*, **2016**, 116, 3540-93	68.1	291
204	Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution. *Journal of Chemical Physics*, **2007**, 126, 184102	3.9	271
203	Absorption and fluorescence spectra of uracil in the gas phase and in aqueous solution: a TD-DFT quantum mechanical study. *Journal of the American Chemical Society*, **2004**, 126, 14320-1	16.4	172
202	Absolute pKa determination for carboxylic acids using density functional theory and the polarizable continuum model. *Chemical Physics Letters*, **2003**, 373, 411-415	2.5	168
201	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
200	DNA/RNA: Building Blocks of Life Under UV Irradiation. *Journal of Physical Chemistry Letters*, **2010**, 1, 2025-2030	6.4	159
199	Ab initio calculations of absorption spectra of large molecules in solution: coumarin C153. *Angewandte Chemie - International Edition*, **2007**, 46, 405-8	16.4	157
198	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
197	Solvent effect on the singlet excited-state lifetimes of nucleic acid bases: A computational study of 5-fluorouracil and uracil in acetonitrile and water. *Journal of the American Chemical Society*, **2006**, 128, 16312-22	16.4	142
196	Understanding the role of stereoelectronic effects in determining collagen stability. 1. A quantum mechanical study of proline, hydroxyproline, and fluoroproline dipeptide analogues in aqueous solution. *Journal of the American Chemical Society*, **2001**, 123, 12568-77	16.4	125
195	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

194	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
193	Structure and conformational behavior of biopolymers by density functional calculations employing periodic boundary conditions. I. The case of polyglycine, polyalanine, and poly-alpha-aminoisobutyric acid in vacuo. *Journal of the American Chemical Society*, **2001**, 123, 3311-22	16.4	115
192	UV-Induced Proton Transfer between DNA Strands. *Journal of the American Chemical Society*, **2015**, 137, 7059-62	16.4	103
191	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
190	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
189	Singlet excited state dynamics of uracil and thymine derivatives: A femtosecond fluorescence upconversion study in acetonitrile. *Chemical Physics Letters*, **2006**, 429, 551-557	2.5	90
188	Excited-state behavior of trans and cis isomers of stilbene and stiff stilbene: a TD-DFT study. *Journal of Physical Chemistry A*, **2005**, 109, 10058-67	2.8	88
187	Checking the pH-induced conformational transition of prion protein by molecular dynamics simulations: effect of protonation of histidine residues. *Biophysical Journal*, **2004**, 87, 3623-32	2.9	88
186	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
185	Quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuum and in aqueous solution. *Journal of Computational Chemistry*, **2002**, 23, 341-50	3.5	79
184	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
183	Solvent Polarity and pH Effects on the Magnetic Properties of Ionizable Nitroxide Radicals: A Combined Computational and Experimental Study of 2,2,5,5-Tetramethyl-3-carboxypyrrolidine and 2,2,6,6-Tetramethyl-4-carboxypiperidine Nitroxides. *Journal of Physical Chemistry A*, **2002**, 106, 10700-10706	2.8	77
182	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
181	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. *Journal of Chemical Theory and Computation*, **2007**, 3, 1803-17	6.4	75
180	Solvent effect on the singlet excited-state dynamics of 5-fluorouracil in acetonitrile as compared with water. *Journal of Physical Chemistry B*, **2006**, 110, 12843-7	3.4	73
179	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
178	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
177	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

176	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
175	Understanding the role of stereoelectronic effects in determining collagen stability. 2. A quantum mechanical/molecular mechanical study of (Proline-Proline-Glycine)(n) polypeptides. *Journal of the American Chemical Society*, **2002**, 124, 7857-65	16.4	63
174	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
173	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
172	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
171	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
170	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
169	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
168	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
167	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
166	Assessing the reliability of density functional methods in the conformational study of polypeptides: the treatment of intraresidue nonbonding interactions. *Journal of Computational Chemistry*, **2004**, 25, 1333-41	3.5	54
165	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
164	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
163	The conformational behavior of polyglycine as predicted by a density functional model with periodic boundary conditions. *Journal of Chemical Physics*, **2001**, 114, 2541-2549	3.9	52
162	Solvent effects on electron-driven proton-transfer processes: adenine-thymine base pairs. *Physical Chemistry Chemical Physics*, **2012**, 14, 8981-9	3.6	51
161	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
160	Computation of protein pK□ values by an integrated density functional theory/Polarizable Continuum Model approach. *Theoretical Chemistry Accounts*, **2004**, 111, 237-245	1.9	51
159	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

158	Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods. *International Journal of Mass Spectrometry*, **2000**, 201, 321-336	1.9	50
157	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
156	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
155	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
154	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
153	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
152	Assessing the acid-base and conformational properties of histidine residues in human prion protein (125-228) by means of pK(a) calculations and molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 167-77	4.2	44
151	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. *Journal of Physical Chemistry Letters*, **2017**, 8, 1777-1783	6.4	43
150	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
149	Computational design, synthesis, and mechanochromic properties of new thiophene-based π-conjugated chromophores. *Chemistry - A European Journal*, **2013**, 19, 1996-2004	4.8	41
148	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
147	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. *Physical Chemistry Chemical Physics*, **2010**, 12, 10550-61	3.6	41
146	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
145	The interplay between π/nπ excited states in gas-phase thymine: a quantum dynamical study. *ChemPhysChem*, **2011**, 12, 1957-68	3.2	39
144	Time dependent DFT investigation on the two lowest 1Bu states of the trans isomer of stilbene and stiff-stilbenes. *Chemical Physics Letters*, **2004**, 387, 509-516	2.5	39
143	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
142	Role of side chains in collagen triple helix stabilization and partner recognition. *Journal of Peptide Science*, **2009**, 15, 131-40	2.1	38
141	A Theoretical Study on the Factors Influencing Cyanine Photoisomerization: The Case of Thiacyanine in Gas Phase and in Methanol. *Journal of Chemical Theory and Computation*, **2005**, 1, 215-29	6.4	38

140	Quantum mechanical prediction of the magnetic titration curve of a nitroxide 'spin probe'. *Chemical Physics Letters*, **2001**, 336, 349-356	2.5	38
139	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
138	Torsional Barriers and Correlations between Dihedrals inp-Polyphenyls. *Journal of Physical Chemistry A*, **2003**, 107, 8665-8670	2.8	37
137	Structure and magnetic properties of nitroxide molecular crystals by density functional calculations employing periodic boundary conditions. *Journal of the American Chemical Society*, **2002**, 124, 113-20	16.4	37
136	Polymerization Mechanism of Conjugated Dienes in the Presence of ZieglerNatta Type Catalysts: Theoretical Study of Butadiene and Isoprene Polymerization with CpTiCl3MAO Initiator. *Organometallics*, **2000**, 19, 411-419	3.8	37
135	Excited states behavior of nucleobases in solution: insights from computational studies. *Topics in Current Chemistry*, **2015**, 355, 329-57		36
134	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
133	Mechanism of Isoprene and Butadiene Polymerization in the Presence of CpTiCl3MAO Initiator: A Theoretical Study. *Macromolecules*, **1997**, 30, 2219-2227	5.5	35
132	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
131	Peptide bond distortions from planarity: new insights from quantum mechanical calculations and peptide/protein crystal structures. *PLoS ONE*, **2011**, 6, e24533	3.7	35
130	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
129	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
128	Optical Properties of Guanine Nanowires: Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2010**, 114, 14339-14346	3.8	34
127	Conformational and spectroscopic analysis of the tyrosyl radical dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model. *Journal of the American Chemical Society*, **2002**, 124, 11531-40	16.4	34
126	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
125	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
124	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
123	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

122	Excited-State Dynamics of DNA Duplexes with Different H-Bonding Motifs. *Journal of Physical Chemistry Letters*, **2016**, 7, 950-4	6.4	30
121	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
120	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
119	Contribution of dipole-dipole interactions to the stability of the collagen triple helix. *Protein Science*, **2008**, 17, 955-61	6.3	29
118	Conformational Behavior of Macromolecules in Solution. Homopolypeptides of □Aminoisobutyric Acid as Test Cases. *Macromolecules*, **2001**, 34, 7550-7557	5.5	29
117	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
116	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
115	Understanding electron transfer across negatively-charged Aib oligopeptides. *Journal of Physical Chemistry B*, **2005**, 109, 1023-33	3.4	28
114	Conformational analysis of the tyrosine dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model. *Journal of Computational Chemistry*, **2002**, 23, 650-61	3.5	28
113	Effective modeling of intrinsic and environmental effects on the structure and electron paramagnetic resonance parameters of nitroxides by an integrated quantum mechanical/molecular mechanics/polarizable continuum model approach. *Theoretical Chemistry Accounts*, **2000**, 104, 273-279	1.9	28
112	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
111	Femtosecond photoelectron spectroscopy of trans-stilbene above the reaction barrier. *Chemical Physics*, **2005**, 310, 201-211	2.3	27
110	Femtosecond study on the isomerization dynamics of NK88. II. Excited-state dynamics. *Journal of Chemical Physics*, **2006**, 125, 44513	3.9	26
109	Does tetracycline bind helix 2 of prion? An integrated spectroscopical and computational study of the interaction between the antibiotic and alpha helix 2 human prion protein fragments. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 707-15	4.2	26
108	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
107	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
106	Femtosecond study on the isomerization dynamics of NK88. I. Ground-state dynamics after photoexcitation. *Journal of Chemical Physics*, **2006**, 125, 44512	3.9	25
105	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

104	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
103	Adenine radicals generated in alternating AT duplexes by direct absorption of low-energy UV radiation. *Faraday Discussions*, **2018**, 207, 181-197	3.6	23
102	Photoinduced long-lived charge transfer excited states in AT-DNA strands. *Physical Chemistry Chemical Physics*, **2016**, 18, 21241-5	3.6	23
101	Conformational Behavior and Magnetic Properties of a Nitroxide Amino Acid Derivative in Vacuo and in Aqueous Solution. *Journal of Physical Chemistry A*, **2003**, 107, 6264-6269	2.8	23
100	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
99	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
98	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
97	Computation of Spectroscopic Parameters in vacuo and in Condensed Phases by Methods based on the Density Functional Theory. *QSAR and Combinatorial Science*, **2002**, 21, 105-118		21
96	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The □/n□ Decay of Thymine in Water as a Test Case. *Journal of Chemical Theory and Computation* , **2018**, 14, 820-832	6.4	20
95	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
94	Parametrization and Validation of Coarse Grained Force-Fields Derived from ab Initio Calculations. *Journal of Chemical Theory and Computation*, **2006**, 2, 556-67	6.4	19
93	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
92	Comprehensive Study of Guanine Excited State Relaxation and Photoreactivity in G-quadruplexes. *Journal of Physical Chemistry Letters*, **2019**, 10, 6873-6877	6.4	18
91	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
90	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
89	Benzophenone photophore flexibility and proximity: molecular and crystal-state structure of a Bpa-containing trichogin dodecapeptide analogue. *ChemBioChem*, **2004**, 5, 541-4	3.8	18
88	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
87	Excited State Pathways Leading to Formation of Adenine Dimers. *Journal of Physical Chemistry Letters*, **2016**, 7, 2020-3	6.4	18

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85	Building cavities in a fluid of spherical or rod-like particles: a contribution to the solvation free energy in isotropic and anisotropic polarizable continuum model. *Journal of Computational Chemistry*, **2005**, 26, 1096-105	3.5	17
84	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
83	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
82	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
81	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
80	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
79	A polarizable continuum approach for the study of heterogeneous dielectric environments. *Journal of Chemical Physics*, **2006**, 124, 184103	3.9	16
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77	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
76	A parameter-free quantum-mechanical approach for calculating electron-transfer rates for large systems in solution. *ChemPhysChem*, **2006**, 7, 1211-4	3.2	15
75	Radicals Generated in Tetramolecular Guanine Quadruplexes by Photoionization: Spectral and Dynamical Features. *Journal of Physical Chemistry B*, **2019**, 123, 4950-4957	3.4	14
74	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
73	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
72	Nucleophilic cyclopropane ring opening in duocarmycin SA derivatives by methanol under acid conditions: a quantum mechanical study in the gas-phase and in solution. *Journal of Organic Chemistry*, **2004**, 69, 2816-24	4.2	14
71	Predicting light absorption properties of anthocyanidins in solution: a multi-level computational approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
70	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
69	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

68	The Influence of Back-Biting Interaction on the Polymerization of Conjugated Dienes in the Presence of Ziegler Natta Catalysts. *Macromolecules*, **1999**, 32, 6852-6855	5.5	13
67	Photoactivated proton coupled electron transfer in DNA: insights from quantum mechanical calculations. *Faraday Discussions*, **2018**, 207, 199-216	3.6	12
66	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
65	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
64	UV-light-induced hydrogen transfer in guanosine-guanosine aggregates. *Chemistry - A European Journal*, **2013**, 19, 5425-31	4.8	11
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