Artur Nenov

List of Publications by Citations

77 papers	2,489 citations	24 h-index	48 g-index
88 ext. papers	3,013 ext. citations	4.9 avg, IF	4.86 L-index

#	Paper	IF	Citations
77	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
76	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
75	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in trans-Azobenzene. *Journal of Physical Chemistry Letters*, **2018**, 9, 1534-1541	6.4	76
74	Making fast photoswitches faster--using Hammett analysis to understand the limit of donor-acceptor approaches for faster hemithioindigo photoswitches. *Chemistry - A European Journal*, **2014**, 20, 13984-92	4.8	55
73	Molecular driving forces for Z/E isomerization mediated by heteroatoms: the example hemithioindigo. *Journal of Physical Chemistry A*, **2010**, 114, 13016-30	2.8	51
72	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
71	Beyond the van der Lugt/Oosterhoff model: when the conical intersection seam and the S1 minimum energy path do not cross. *Journal of Organic Chemistry*, **2010**, 75, 123-9	4.2	46
70	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. *Journal of Physical Chemistry Letters*, **2017**, 8, 1777-1783	6.4	43
69	Observation of the Sub-100 Femtosecond Population of a Dark State in a Thiobase Mediating Intersystem Crossing. *Journal of the American Chemical Society*, **2018**, 140, 16087-16093	16.4	39
68	Accelerated and efficient photochemistry from higher excited electronic states in fulgide molecules. *Journal of Physical Chemistry A*, **2008**, 112, 13364-71	2.8	38
67	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. *Journal of Chemical Physics*, **2015**, 142, 212443	3.9	37
66	Spectral lineshapes in nonlinear electronic spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 30925-36	3.6	34
65	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. *International Journal of Quantum Chemistry*, **2014**, 114, 85-93	2.1	34
64	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
63	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
62	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. *Physical Chemistry Chemical Physics*, **2015**, 17, 7291-302	3.6	31
61	Disentangling Peptide Configurations via Two-Dimensional Electronic Spectroscopy: Ab Initio Simulations Beyond the Frenkel Exciton Hamiltonian. *Journal of Physical Chemistry Letters*, **2014**, 5, 767-771	6.4	31

60	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. *Physical Chemistry Chemical Physics*, **2014**, 16, 16865-79	3.6	30
59	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. *Journal of Molecular Modeling*, **2018**, 24, 271	2	29
58	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. *Photochemical and Photobiological Sciences*, **2015**, 14, 213-28	4.2	27
57	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. *Faraday Discussions*, **2015**, 177, 345-62	3.6	27
56	Modelling time-resolved two-dimensional electronic spectroscopy of the primary photoisomerization event in rhodopsin. *Journal of Physical Chemistry B*, **2014**, 118, 8396-405	3.4	27
55	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. *Chemistry - A European Journal*, **2016**, 22, 7497-507	4.8	26
54	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	24
53	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. *Chemical Science*, **2019**, 10, 9907-9921	9.4	24
52	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. *Journal of Chemical Theory and Computation*, **2015**, 11, 3755-71	6.4	23
51	Multidimensional Potential Energy Surfaces Resolved at the RASPT2 Level for Accurate Photoinduced Isomerization Dynamics of Azobenzene. *Journal of Chemical Theory and Computation*, **2019**, 15, 6813-6823	6.4	23
50	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. *Frontiers in Chemistry*, **2015**, 3, 29	5	23
49	Ultrafast Spectroscopy of Photoactive Molecular Systems from First Principles: Where We Stand Today and Where We Are Going. *Journal of the American Chemical Society*, **2020**, 142, 16117-16139	16.4	23
48	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. *Journal of Physical Chemistry Letters*, **2019**, 10, 3481-3487	6.4	22
47	Tracking conformational dynamics of polypeptides by nonlinear electronic spectroscopy of aromatic residues: a first-principles simulation study. *ChemPhysChem*, **2014**, 15, 3282-90	3.2	22
46	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 295-303	2	20
45	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landau-Zener Model. *Journal of Physical Chemistry Letters*, **2018**, 9, 3315-3322	6.4	20
44	Molecular model of the ring-opening and ring-closure reaction of a fluorinated indolylfulgide. *Journal of Physical Chemistry A*, **2012**, 116, 10518-28	2.8	17
43	Geometrical and substituent effects in conical intersections: linking chemical structure and photoreactivity in polyenes. *Journal of Chemical Physics*, **2011**, 135, 034304	3.9	17

42	A Unified Experimental/Theoretical Description of the Ultrafast Photophysics of Single and Double Thionated Uracils. *Chemistry - A European Journal*, **2020**, 26, 336-343	4.8	17
41	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. *Faraday Discussions*, **2019**, 221, 219-244	3.6	17
40	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry*, **2018**, 376, 24	7.2	16
39	Photoinduced formation mechanism of the thymine-thymine (6-4) adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study. *Faraday Discussions*, **2018**, 207, 375-387	3.6	15
38	Imaging conical intersection dynamics during azobenzene photoisomerization by ultrafast X-ray diffraction. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	14
37	Anilino-Substituted Multicyanobuta-1,3-diene Electron Acceptors: TICT Molecules with Accessible Conical Intersections. *Journal of Physical Chemistry A*, **2015**, 119, 10677-83	2.8	13
36	Boron-Doped Polycyclic Aromatic Hydrocarbons: A Molecular Set Revealing the Interplay between Topology and Singlet Fission Propensity. *Journal of Physical Chemistry Letters*, **2020**, 11, 1390-1396	6.4	13
35	Linear absorption spectra of solvated thiouracils resolved at the hybrid RASPT2/MM level. *Chemical Physics*, **2018**, 515, 643-653	2.3	13
34	Exploring the capabilities of optical pump X-ray probe NEXAFS spectroscopy to track photo-induced dynamics mediated by conical intersections. *Faraday Discussions*, **2019**, 221, 245-264	3.6	12
33	Intramolecular photo-induced charge transfer in visual retinal chromophore mimics: electron density-based indices at the TD-DFT and post-HF levels. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
32	On the Simulation of Two-dimensional Electronic Spectroscopy of Indole-containing Peptides. *Photochemistry and Photobiology*, **2017**, 93, 1368-1380	3.6	10
31	X-ray linear and non-linear spectroscopy of the ESCA molecule. *Journal of Chemical Physics*, **2019**, 151, 114110	3.9	10
30	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
29	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. *Faraday Discussions*, **2018**, 207, 233-250	3.6	10
28	Conical intersection seams in polyenes derived from their chemical composition. *Journal of Chemical Physics*, **2012**, 137, 074101	3.9	10
27	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
26	Dynamics of chemical bond: general discussion. *Faraday Discussions*, **2015**, 177, 121-54	3.6	8
25	Spectral Tuning and Photoisomerization Efficiency in Push-Pull Azobenzenes: Designing Principles. *Journal of Physical Chemistry A*, **2020**, 124, 9513-9523	2.8	8

24	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. *Journal of Physical Chemistry B*, **2018**, 122, 7668-7681	3.4	7
23	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. *ChemPhotoChem*, **2019**, 3, 107-116	3.3	7
22	Parameterization of a linear vibronic coupling model with multiconfigurational electronic structure methods to study the quantum dynamics of photoexcited pyrene. *Journal of Chemical Physics*, **2021**, 154, 104106	3.9	6
21	iSPECTRON: A simulation interface for linear and nonlinear spectra with ab-initio quantum chemistry software. *Journal of Computational Chemistry*, **2021**, 42, 644-659	3.5	6
20	Photoelectrochromism in the Retinal Protonated Schiff Base Chromophore: Photoisomerization Speed and Selectivity under a Homogeneous Electric Field at Different Operational Regimes. *Journal of Chemical Theory and Computation*, **2016**, 12, 4460-75	6.4	5
19	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
18	Future challenges: general discussion. *Faraday Discussions*, **2015**, 177, 517-45	3.6	3
17	Impacts of hydroxylation on the photophysics of chalcones: insights into the relation between the chemical composition and the electronic structure. *Physical Chemistry Chemical Physics*, **2018**, 20, 8924-8934	3.6	3
16	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time		3
15	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry Collections*, **2019**, 63-112	1.8	3
14	Tailored Coumarin Dyes for Photoredox Catalysis: Calculation, Synthesis, and Electronic Properties. *ChemCatChem*, **2021**, 13, 981-989	5.2	3
13	Manipulating Core Excitations in Molecules by X-Ray Cavities. *Physical Review Letters*, **2021**, 126, 053201	7.4	3
12	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time.. *Nature Communications*, **2021**, 12, 7285	17.4	3
11	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. *Journal of Chemical Theory and Computation*, **2021**, 17, 7134-7145	6.4	2
10	Intersystem crossing in thiobases proceeds by a dark intermediate state. *EPJ Web of Conferences*, **2019**, 205, 10005	0.3	1
9	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. *Angewandte Chemie - International Edition*, **2020**, 59, 20619-20627	16.4	1
8	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. *Molecules*, **2021**, 26,	4.8	1
7	Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12300-12309	6.4	1

6	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 77-142	0.7	0
5	UV-light induced vibrational coherences explain Kasha rule violation in frans-azobenzene. *EPJ Web of Conferences*, **2019**, 205, 09016	0.3	
4	Conical intersection dynamics of pyrimidine nucleosides tracked with sub-20-fs UV pulses. *EPJ Web of Conferences*, **2019**, 205, 10007	0.3	
3	Local and Global Dynamics: general discussion. *Faraday Discussions*, **2015**, 177, 381-403	3.6	
2	Tuning of Isomerization Rates in Indigo-Based Photoswitches. *Springer Proceedings in Physics*, **2015**, 391-394	0.4	
1	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. *Angewandte Chemie*, **2020**, 132, 20800-20808	3.6	