Artur Nenov

List of Publications by Year in descending order

86 papers	3,541 citations	172207 29 h-index	143772 57 g-index
88 all docs	88 docs citations	88 times ranked	3443 citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
2	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
3	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in trans-Azobenzene. Journal of Physical Chemistry Letters, 2018, 9, 1534-1541.	2.1	96
4	Making Fast Photoswitches Fasterâ€"Using Hammett Analysis to Understand the Limit of Donorâ€"Acceptor Approaches for Faster Hemithioindigo Photoswitches. Chemistry - A European Journal, 2014, 20, 13984-13992.	1.7	78
5	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.	6.6	76
6	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.	6.6	63
7	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. Journal of Physical Chemistry Letters, 2017, 8, 1777-1783.	2.1	60
8	Molecular Driving Forces for Z/E Isomerization Mediated by Heteroatoms: The Example Hemithioindigo. Journal of Physical Chemistry A, 2010, 114, 13016-13030.	1.1	58
9	COBRAMM 2.0 â€" A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. Journal of Molecular Modeling, 2018, 24, 271.	0.8	55
10	Beyond the van der Lugt/Oosterhoff Model: When the Conical Intersection Seam and the S₁Minimum Energy Path Do Not Cross. Journal of Organic Chemistry, 2010, 75, 123-129.	1.7	52
11	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. Physical Chemistry Chemical Physics, 2018, 20, 6877-6890.	1.3	46
12	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. Journal of Chemical Physics, 2015, 142, 212443.	1.2	44
13	Accelerated and Efficient Photochemistry from Higher Excited Electronic States in Fulgide Molecules. Journal of Physical Chemistry A, 2008, 112, 13364-13371.	1.1	41
14	Multiple Electronic and Structural Factors Control Cyclobutane Pyrimidine Dimer and 6â€"4 Thymineâ€"Thymine Photodimerization in a DNA Duplex. Chemistry - A European Journal, 2017, 23, 15177-15188.	1.7	41
15	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. Chemical Science, 2019, 10, 9907-9921.	3.7	40
16	Spectral lineshapes in nonlinear electronic spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 30925-30936.	1.3	39
17	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.	2.3	39
18	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.	6.6	39

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19	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. International Journal of Quantum Chemistry, 2014, 114, 85-93.	1.0	38
20	Modelling Time-Resolved Two-Dimensional Electronic Spectroscopy of the Primary Photoisomerization Event in Rhodopsin. Journal of Physical Chemistry B, 2014, 118, 8396-8405.	1.2	35
21	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, 7291-7302.	1.3	35
22	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. Photochemical and Photobiological Sciences, 2015, 14, 213-228.	1.6	35
23	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. Journal of Physical Chemistry Letters, 2019, 10, 3481-3487.	2.1	35
24	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.	2.1	34
25	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. Physical Chemistry Chemical Physics, 2014, 16, 16865-16879.	1.3	33
26	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time. Nature Communications, 2021, 12, 7285.	5.8	32
27	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. Frontiers in Chemistry, 2015, 3, 29.	1.8	31
28	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	1.7	31
29	A Unified Experimental/Theoretical Description of the Ultrafast Photophysics of Single and Double Thionated Uracils. Chemistry - A European Journal, 2020, 26, 336-343.	1.7	31
30	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, .	3.3	31
31	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. Faraday Discussions, 2015, 177, 345-362.	1.6	29
32	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	28
33	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landauâ€“Zener Model. Journal of Physical Chemistry Letters, 2018, 9, 3315-3322.	2.1	28
34	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. Journal of Chemical Theory and Computation, 2015, 11, 3755-3771.	2.3	27
35	Spectral Tuning and Photoisomerization Efficiency in Pushâ€“Pull Azobenzenes: Designing Principles. Journal of Physical Chemistry A, 2020, 124, 9513-9523.	1.1	27
36	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.	1.6	25

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37	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. Faraday Discussions, 2019, 221, 219-244.	1.6	24
38	Tracking Conformational Dynamics of Polypeptides by Nonlinear Electronic Spectroscopy of Aromatic Residues: A Firstâ€Principles Simulation Study. ChemPhysChem, 2014, 15, 3282-3290.	1.0	23
39	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry, 2018, 376, 24.	3.0	23
40	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. Computational and Theoretical Chemistry, 2014, 1040-1041, 295-303.	1.1	21
41	Anilino-Substituted Multicyanobuta-1,3-diene Electron Acceptors: TICT Molecules with Accessible Conical Intersections. Journal of Physical Chemistry A, 2015, 119, 10677-10683.	1.1	21
42	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.	2.1	21
43	Photoinduced formation mechanism of the thymineâ€“thymine (6â€“4) adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study. Faraday Discussions, 2018, 207, 375-387.	1.6	20
44	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.	1.2	20
45	Molecular Model of the Ring-Opening and Ring-Closure Reaction of a Fluorinated Indolylfulgide. Journal of Physical Chemistry A, 2012, 116, 10518-10528.	1.1	19
46	Linear absorption spectra of solvated thiouracils resolved at the hybrid RASPT2/MM level. Chemical Physics, 2018, 515, 643-653.	0.9	19
47	X-ray linear and non-linear spectroscopy of the ESCA molecule. Journal of Chemical Physics, 2019, 151, 114110.	1.2	19
48	Geometrical and substituent effects in conical intersections: Linking chemical structure and photoreactivity in polyenes. Journal of Chemical Physics, 2011, 135, 034304.	1.2	18
49	Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 12300-12309.	2.1	17
50	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.	0.5	15
51	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
52	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. Faraday Discussions, 2018, 207, 233-250.	1.6	14
53	<scp>iSPECTRON</scp>: A simulation interface for linear and nonlinear spectra with abâ€initio quantum chemistry software. Journal of Computational Chemistry, 2021, 42, 644-659.	1.5	14
54	Automatized protocol and interface to simulate <scp>QM</scp>/<scp>MM timeâ€resolved</scp> transient absorption at <scp>TDâ€DFT</scp> level with <scp>COBRAMM</scp>. Journal of Computational Chemistry, 2022, 43, 1641-1655.	1.5	14

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55	On the Simulation of Twoâ€dimensional Electronic Spectroscopy of Indoleâ€containing Peptides. Photochemistry and Photobiology, 2017, 93, 1368-1380.	1.3	13
56	Manipulating Core Excitations in Molecules by X-Ray Cavities. Physical Review Letters, 2021, 126, 053201.	2.9	13
57	Conical intersection seams in polyenes derived from their chemical composition. Journal of Chemical Physics, 2012, 137, 074101.	1.2	11
58	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, 4460-4475.	2.3	11
59	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. ChemPhotoChem, 2019, 3, 107-116.	1.5	11
60	Soft X-ray Spectroscopy Simulations with Multiconfigurational Wave Function Theory: Spectrum Completeness, Sub-eV Accuracy, and Quantitative Reproduction of Line Shapes. Journal of Chemical Theory and Computation, 2022, 18, 1003-1016.	2.3	11
61	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	1.6	10
62	Tailored Coumarin Dyes for Photoredox Catalysis: Calculation, Synthesis, and Electronic Properties. ChemCatChem, 2021, 13, 981-989.	1.8	10
63	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. Angewandte Chemie - International Edition, 2020, 59, 20619-20627.	7.2	9
64	Dynamics of chemical bond: general discussion. Faraday Discussions, 2015, 177, 121-154.	1.6	8
65	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. Journal of Physical Chemistry B, 2018, 122, 7668-7681.	1.2	8
66	Environment-Driven Coherent Population Transfer Governs the Ultrafast Photophysics of Tryptophan. Journal of the American Chemical Society, 2022, 144, 12884-12892.	6.6	8
67	Photoisomerization transition state manipulation by entangled two-photon absorption. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	7
68	Time-Resolved Optical Pump-Resonant X-ray Probe Spectroscopy of 4-Thiouracil: A Simulation Study. Journal of Chemical Theory and Computation, 2022, 18, 3075-3088.	2.3	7
69	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. Journal of Chemical Theory and Computation, 2021, 17, 7134-7145.	2.3	6
70	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
71	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.	1.3	5
72	Coupled Electronic and Nuclear Motions during Azobenzene Photoisomerization Monitored by Ultrafast Electron Diffraction. Journal of Chemical Theory and Computation, 2022, 18, 605-613.	2.3	5

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73	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry Collections, 2019, , 63-112.	0.2	4
74	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. Challenges and Advances in Computational Chemistry and Physics, 2021, , 77-142.	0.6	4
75	Future challenges: general discussion. Faraday Discussions, 2015, 177, 517-545.	1.6	3
76	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. Molecules, 2021, 26, 396.	1.7	2
77	Intersystem crossing in thiobases proceeds by a dark intermediate state. EPJ Web of Conferences, 2019, 205, 10005.	0.1	1
78	Local and Global Dynamics: general discussion. Faraday Discussions, 2015, 177, 381-403.	1.6	0
79	Tracking azobenzene photoisomerization with sub-20-fs UV pulses. , 2017, , .		0
80	Conical Intersection Dynamics of Pyrimidine Nucleosides Tracked with Sub-20-fs UV Pulses. , 2019, , .		0
81	UV-light induced vibrational coherences explain Kasha rule violation in frans-azobenzene. EPJ Web of Conferences, 2019, 205, 09016.	0.1	0
82	Conical intersection dynamics of pyrimidine nucleosides tracked with sub-20-fs UV pulses. EPJ Web of Conferences, 2019, 205, 10007.	0.1	0
83	Sub-20 fs UV spectroscopy to track primary photoinduced processes in Thiobases. , 2019, , .		0
84	Intersystem Crossing in Thiobases Proceeds by a Dark Intermediate State. , 2019, , .		0
85	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. Angewandte Chemie, 2020, 132, 20800-20808.	1.6	0
86	Monitoring Ultrafast Photoisomerization of Azobenzene by Time-Resolved X-Ray Diffraction. , 2020, , .		0