

Artur Nenov

List of Publications by Year in descending order

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3,541
citations

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#	ARTICLE	IF	CITATIONS
1	Soft X-ray Spectroscopy Simulations with Multiconfigurational Wave Function Theory: Spectrum Completeness, Sub-eV Accuracy, and Quantitative Reproduction of Line Shapes. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1003-1016.	5.3	11
2	Coupled Electronic and Nuclear Motions during Azobenzene Photoisomerization Monitored by Ultrafast Electron Diffraction. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 605-613.	5.3	5
3	Time-Resolved Optical Pump-Resonant X-ray Probe Spectroscopy of 4-Thiouracil: A Simulation Study. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3075-3088.	5.3	7
4	Automatized protocol and interface to simulate QM/MM time-resolved transient absorption at $TD\text{-}DFT$ level with $COBRAMM$. <i>Journal of Computational Chemistry</i> , 2022, 43, 1641-1655.	3.3	14
5	Environment-Driven Coherent Population Transfer Governs the Ultrafast Photophysics of Tryptophan. <i>Journal of the American Chemical Society</i> , 2022, 144, 12884-12892.	13.7	8
6	Tailored Coumarin Dyes for Photoredox Catalysis: Calculation, Synthesis, and Electronic Properties. <i>ChemCatChem</i> , 2021, 13, 981-989.	3.7	10
7	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. <i>Molecules</i> , 2021, 26, 396.	3.8	2
8	$iSPECTRON$: A simulation interface for linear and nonlinear spectra with <i>ab initio</i> quantum chemistry software. <i>Journal of Computational Chemistry</i> , 2021, 42, 644-659.	3.3	14
9	Manipulating Core Excitations in Molecules by X-Ray Cavities. <i>Physical Review Letters</i> , 2021, 126, 053201.	7.8	13
10	Parameterization of a linear vibronic coupling model with multiconfigurational electronic structure methods to study the quantum dynamics of photoexcited pyrene. <i>Journal of Chemical Physics</i> , 2021, 154, 104106.	3.0	20
11	Imaging conical intersection dynamics during azobenzene photoisomerization by ultrafast X-ray diffraction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	31
12	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7134-7145.	5.3	6
13	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021, , 77-142.	0.6	4
14	Photoisomerization transition state manipulation by entangled two-photon absorption. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	7
15	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time. <i>Nature Communications</i> , 2021, 12, 7285.	12.8	32
16	Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12300-12309.	4.6	17
17	A Unified Experimental/Theoretical Description of the Ultrafast Photophysics of Single and Double Thionated Uracils. <i>Chemistry - A European Journal</i> , 2020, 26, 336-343.	3.3	31
18	Spectral Tuning and Photoisomerization Efficiency in Push-Pull Azobenzenes: Designing Principles. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9513-9523.	2.5	27

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19	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20619-20627.	13.8	9
20	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. <i>Angewandte Chemie</i> , 2020, 132, 20800-20808.	2.0	0
21	Ultrafast Spectroscopy of Photoactive Molecular Systems from First Principles: Where We Stand Today and Where We Are Going. <i>Journal of the American Chemical Society</i> , 2020, 142, 16117-16139.	13.7	39
22	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020, 152, 214117.	3.0	281
23	Boron-Doped Polycyclic Aromatic Hydrocarbons: A Molecular Set Revealing the Interplay between Topology and Singlet Fission Propensity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1390-1396.	4.6	21
24	Monitoring Ultrafast Photoisomerization of Azobenzene by Time-Resolved X-Ray Diffraction. , 2020, , .		0
25	Multidimensional Potential Energy Surfaces Resolved at the RASPT2 Level for Accurate Photoinduced Isomerization Dynamics of Azobenzene. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6813-6823.	5.3	39
26	Conical Intersection Dynamics of Pyrimidine Nucleosides Tracked with Sub-20-fs UV Pulses. , 2019, , .		0
27	UV-light induced vibrational coherences explain Kasha rule violation in trans-azobenzene. <i>EPJ Web of Conferences</i> , 2019, 205, 09016.	0.3	0
28	Intersystem crossing in thiobases proceeds by a dark intermediate state. <i>EPJ Web of Conferences</i> , 2019, 205, 10005.	0.3	1
29	Conical intersection dynamics of pyrimidine nucleosides tracked with sub-20-fs UV pulses. <i>EPJ Web of Conferences</i> , 2019, 205, 10007.	0.3	0
30	X-ray linear and non-linear spectroscopy of the ESCA molecule. <i>Journal of Chemical Physics</i> , 2019, 151, 114110.	3.0	19
31	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3481-3487.	4.6	35
32	Sub-20 fs UV spectroscopy to track primary photoinduced processes in Thiobases. , 2019, , .		0
33	Intersystem Crossing in Thiobases Proceeds by a Dark Intermediate State. , 2019, , .		0
34	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. <i>Chemical Science</i> , 2019, 10, 9907-9921.	7.4	40
35	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. <i>ChemPhotoChem</i> , 2019, 3, 107-116.	3.0	11
36	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. <i>Topics in Current Chemistry Collections</i> , 2019, , 63-112.	0.5	4

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37	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. <i>Faraday Discussions</i> , 2019, 221, 219-244.	3.2	24
38	Exploring the capabilities of optical pump X-ray probe NEXAFS spectroscopy to track photo-induced dynamics mediated by conical intersections. <i>Faraday Discussions</i> , 2019, 221, 245-264.	3.2	25
39	Impacts of hydroxylation on the photophysics of chalcones: insights into the relation between the chemical composition and the electronic structure. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8924-8934.	2.8	5
40	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	14
41	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in <i>trans</i> -Azobenzene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1534-1541.	4.6	96
42	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6877-6890.	2.8	46
43	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 323-331.	2.9	10
44	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. <i>Faraday Discussions</i> , 2018, 207, 233-250.	3.2	14
45	Photoinduced formation mechanism of the thymine-thymine (6 ⁴) adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study. <i>Faraday Discussions</i> , 2018, 207, 375-387.	3.2	20
46	Observation of the Sub-100 Femtosecond Population of a Dark State in a Thiobase Mediating Intersystem Crossing. <i>Journal of the American Chemical Society</i> , 2018, 140, 16087-16093.	13.7	63
47	COBRAMM 2.0 – A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. <i>Journal of Molecular Modeling</i> , 2018, 24, 271.	1.8	55
48	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landau-Zener Model. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3315-3322.	4.6	28
49	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7668-7681.	2.6	8
50	Linear absorption spectra of solvated thiouracils resolved at the hybrid RASPT2/MM level. <i>Chemical Physics</i> , 2018, 515, 643-653.	1.9	19
51	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. <i>Topics in Current Chemistry</i> , 2018, 376, 24.	5.8	23
52	Photophysics of Deoxycytidine and 5-Methyldeoxycytidine in Solution: A Comprehensive Picture by Quantum Mechanical Calculations and Femtosecond Fluorescence Spectroscopy. <i>Journal of the American Chemical Society</i> , 2017, 139, 7780-7791.	13.7	76
53	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1777-1783.	4.6	60
54	On the Simulation of Two-Dimensional Electronic Spectroscopy of Indole-containing Peptides. <i>Photochemistry and Photobiology</i> , 2017, 93, 1368-1380.	2.5	13

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55	Multiple Electronic and Structural Factors Control Cyclobutane Pyrimidine Dimer and 6â€“4 Thymineâ€“Thymine Photodimerization in a DNA Duplex. <i>Chemistry - A European Journal</i> , 2017, 23, 15177-15188.	3.3	41
56	Tracking azobenzene photoisomerization with sub-20-fs UV pulses. , 2017, , .		0
57	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
58	Intramolecular photo-induced charge transfer in visual retinal chromophore mimics: electron density-based indices at the TD-DFT and post-HF levels. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	15
59	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	5
60	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	28
61	Photoelectrochromism in the Retinal Protonated Schiff Base Chromophore: Photoisomerization Speed and Selectivity under a Homogeneous Electric Field at Different Operational Regimes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4460-4475.	5.3	11
62	Multiple Decay Mechanisms and 2Dâ€“UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€“Uracil Monophosphate. <i>Chemistry - A European Journal</i> , 2016, 22, 7497-7507.	3.3	31
63	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. <i>Frontiers in Chemistry</i> , 2015, 3, 29.	3.6	31
64	Spectral lineshapes in nonlinear electronic spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30925-30936.	2.8	39
65	Dynamics of chemical bond: general discussion. <i>Faraday Discussions</i> , 2015, 177, 121-154.	3.2	8
66	Local and Global Dynamics: general discussion. <i>Faraday Discussions</i> , 2015, 177, 381-403.	3.2	0
67	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7291-7302.	2.8	35
68	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. <i>Photochemical and Photobiological Sciences</i> , 2015, 14, 213-228.	2.9	35
69	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3755-3771.	5.3	27
70	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. <i>Faraday Discussions</i> , 2015, 177, 345-362.	3.2	29
71	Anilino-Substituted Multicyanobuta-1,3-diene Electron Acceptors: TICT Molecules with Accessible Conical Intersections. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10677-10683.	2.5	21
72	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 142, 212443.	3.0	44

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73	Future challenges: general discussion. Faraday Discussions, 2015, 177, 517-545.	3.2	3
74	Tracking Conformational Dynamics of Polypeptides by Nonlinear Electronic Spectroscopy of Aromatic Residues: A First-Principles Simulation Study. ChemPhysChem, 2014, 15, 3282-3290.	2.1	23
75	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, 13984-13992.	3.3	78
76	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. Computational and Theoretical Chemistry, 2014, 1040-1041, 295-303.	2.5	21
77	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. International Journal of Quantum Chemistry, 2014, 114, 85-93.	2.0	38
78	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. Physical Chemistry Chemical Physics, 2014, 16, 16865-16879.	2.8	33
79	Modelling Time-Resolved Two-Dimensional Electronic Spectroscopy of the Primary Photoisomerization Event in Rhodopsin. Journal of Physical Chemistry B, 2014, 118, 8396-8405.	2.6	35
80	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.	4.6	34
81	Conical intersection seams in polyenes derived from their chemical composition. Journal of Chemical Physics, 2012, 137, 074101.	3.0	11
82	Molecular Model of the Ring-Opening and Ring-Closure Reaction of a Fluorinated Indolyfulgide. Journal of Physical Chemistry A, 2012, 116, 10518-10528.	2.5	19
83	Geometrical and substituent effects in conical intersections: Linking chemical structure and photoreactivity in polyenes. Journal of Chemical Physics, 2011, 135, 034304.	3.0	18
84	Beyond the van der Lugt/Oosterhoff Model: When the Conical Intersection Seam and the S ₁ Minimum Energy Path Do Not Cross. Journal of Organic Chemistry, 2010, 75, 123-129.	3.2	52
85	Molecular Driving Forces for Z/E Isomerization Mediated by Heteroatoms: The Example Hemithioindigo. Journal of Physical Chemistry A, 2010, 114, 13016-13030.	2.5	58
86	Accelerated and Efficient Photochemistry from Higher Excited Electronic States in Fulgide Molecules. Journal of Physical Chemistry A, 2008, 112, 13364-13371.	2.5	41