Dana Nachtigallova

List of Publications by Year
in descending order

88 papers	4,030 citations	147801 31 h-index	123424 61 g-index
90 all docs	90 docs citations	90 times ranked	3788 citing authors

#	Article	IF	Citations
1	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. ACS Nano, 2017, 11, 12402-12410.	14.6	550
2	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21453-21458.	7.1	362
3	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
4	Coordination and siting of Cu+ ions in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 1999, 1, 2019-2026.	2.8	215
5	Excited state dynamics of DNA bases. International Reviews in Physical Chemistry, 2013, 32, 308-342.	2.3	185
6	Coordination of Cu+ and Cu2+ ions in ZSM-5 in the vicinity of two framework Al atoms. Physical Chemistry Chemical Physics, 2001, 3, 1552-1559.	2.8	104
7	Coordination Change of Cu+ Sites in ZSM-5 on Excitation in the Triplet State:â€‰ Understanding of the Photoluminescence Spectra. Journal of Physical Chemistry B, 2000, 104, 1738-1745.	2.6	87
8	Nature of the Cu+â^'NO Bond in the Gas Phase and at Different Types of Cu+Sites in Zeolite Catalysts. Journal of Physical Chemistry B, 2004, 108, 13674-13682.	2.6	86
9	Photodynamics Simulations of Thymine: Relaxation into the First Excited Singlet State. Journal of Physical Chemistry A, 2009, 113, 12686-12693.	2.5	85
10	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145.	2.8	84
11	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255.	2.5	84
12	The vibrational dynamics of carbon monoxide in a confined spaceâ€”CO in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 4849-4852.	2.8	74
13	The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227.	3.3	73
14	Calculations of Site-Specific CO Stretching Frequencies for Copper Carbonyls with the â€œNear Spectroscopic Accuracyâ€•â€‰ CO Interaction with Cu+/MFI. Journal of Physical Chemistry A, 2003, 107, 10381-10388.	2.5	71
15	The decay mechanism of photoexcited guanine â^' A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304.	3.0	70
16	Characterization of the Cu+Sites in High-Silica Zeolites Interacting with the CO Molecule:Â Combined Computational and Experimental Study. Journal of Physical Chemistry B, 2003, 107, 2327-2332.	2.6	69
17	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. Nature Communications, 2018, 9, 2831.	12.8	68
18	Does Stacking Restrain the Photodynamics of Individual Nucleobases?. Journal of the American Chemical Society, 2010, 132, 8261-8263.	13.7	67

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19	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	4.3	57
20	Solvatochromic fluorene-linked nucleoside and DNA as color-changing fluorescent probes for sensing interactions. Chemical Science, 2016, 7, 5775-5785.	7.4	55
21	Computational Study of Extraframework Cu+Sites in Ferrierite:Â Structure, Coordination, and Photoluminescence Spectra. Journal of Physical Chemistry B, 2001, 105, 3510-3517.	2.6	49
22	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	5.5	49
23	Electronic coupling in the excited electronic state of stacked DNA base homodimers. Physical Chemistry Chemical Physics, 2007, 9, 1672.	2.8	48
24	Self-Organization of 1-Methylnaphthalene on the Surface of Artificial Snow Grains: A Combined Experimentalâ€“Computational Approach. Journal of Physical Chemistry A, 2011, 115, 11412-11422.	2.5	43
25	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
26	Unravelling the Open-Shell Character of Peripentacene on Au(111). Journal of Physical Chemistry Letters, 2021, 12, 330-336.	4.6	36
27	Electronic splitting in the excited states of DNA base homodimers and -trimers: an evaluation of short-range and Coulombic interactions. Physical Chemistry Chemical Physics, 2008, 10, 5689.	2.8	35
28	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. Journal of Chemical Physics, 2019, 150, 124302.	3.0	35
29	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. Physical Chemistry Chemical Physics, 2019, 21, 9077-9088.	2.8	34
30	On the Existence of CuI Pairs in ZSM-5â€”A Computational Study. Chemistry - A European Journal, 2002, 8, 2099.	3.3	33
31	Chemistry of Small Organic Molecules on Snow Grains: The Applicability of Artificial Snow for Environmental Studies. Environmental Science & Technology, 2011, 45, 3430-3436.	10.0	33
32	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie - International Edition, 2020, 59, 17594-17599.	13.8	33
33	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669.	13.7	31
34	On-Surface Strain-Driven Synthesis of Nonalternant Non-Benzenoid Aromatic Compounds Containing Four- to Eight-Membered Rings. Journal of the American Chemical Society, 2021, 143, 14694-14702.	13.7	31
35	Theoretical study of the ground and excited states of 7-methyl guanine and 9-methyl guanine: comparison with experiment. Physical Chemistry Chemical Physics, 2006, 8, 3059-3065.	2.8	30
36	Spectroscopic Properties of Naphthalene on the Surface of Ice Grains Revisited: A Combined Experimentalâ€“Computational Approach. Journal of Physical Chemistry A, 2015, 119, 8565-8578.	2.5	30

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37	Singlet L_a and L_b Bands for N-Acenes (N = 2â€“7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306.	5.3	30
38	Localization of Cu+sites and framework Al positions in high-silica zeolites: Combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2004, 6, 2003-2007.	2.8	29
39	Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. Physical Chemistry Chemical Physics, 2010, 12, 5375.	2.8	29
40	Spectroscopic Properties of Benzene at the Airâ€“Ice Interface: A Combined Experimentalâ€“Computational Approach. Journal of Physical Chemistry A, 2014, 118, 7535-7547.	2.5	27
41	Mechanisms of Orthogonal Photodecarbonylation Reactions of 3-Hydroxyflavone-Based Acidâ€“Base Forms. Journal of Organic Chemistry, 2020, 85, 3527-3537.	3.2	27
42	Site-Selective Photochemistry in an Alternating 2-Norbornyl-CO Copolymer: Importance of Stereoelectronic Effects. Journal of the American Chemical Society, 1995, 117, 3946-3951.	13.7	26
43	Resonant Infrared Multiple Photon Dissociation Spectroscopy of Anionic Nucleotide Monophosphate Clusters. Journal of Physical Chemistry B, 2015, 119, 7894-7901.	2.6	25
44	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. Journal of Physical Chemistry C, 2020, 124, 14327-14337.	3.1	25
45	FTIR Study of CO Interactions with Li⁺Ions in Micro- and Mesoporous Matrices:â€‰Coordination and Localization of Li⁺Ions. Journal of Physical Chemistry C, 2007, 111, 11353-11362.	3.1	22
46	Combined Experimental and Theoretical Investigations of Heterogeneous Dual Cation Sites in Cu,M-FER Zeolites. Journal of Physical Chemistry C, 2011, 115, 13312-13321.	3.1	20
47	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. Topics in Current Chemistry, 2014, 356, 1-37.	4.0	20
48	The effect of C5 substitution on the photochemistry of uracil. Physical Chemistry Chemical Physics, 2010, 12, 4924.	2.8	19
49	Characterization of Ag+ Sites in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 2001, 3, 4791-4795.	2.8	18
50	Binding Energies of the Ï€â€Stacked Anisole Dimer: New Molecular Beamâ€“Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6740-6746.	3.3	18
51	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. Journal of Physical Chemistry Letters, 2019, 10, 5592-5597.	4.6	18
52	Photochemistry of 4-Chlorophenol in Liquid and Frozen Aqueous Media Studied by Chemical, Compound-Specific Isotope, and DFT Analyses. Langmuir, 2015, 31, 10743-10750.	3.5	17
53	The photodynamics of 2,4-diaminopyrimidine in comparison with 4-aminopyrimidine: The effect of amino-substitution. Chemical Physics Letters, 2010, 497, 129-134.	2.6	16
54	Photodissociation of aniline Nâ€“H bonds in clusters of different nature. Physical Chemistry Chemical Physics, 2015, 17, 25004-25013.	2.8	15

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55	On-Surface Hydrogenation of Buckybowls: From Curved Aromatic Molecules to Planar Non-KekulÃ© Aromatic Hydrocarbons. ACS Nano, 2020, 14, 16735-16742.	14.6	15
56	The Existence of a Nâ†'C Dative Bond in the C₆₀â€"Piperidine Complex. Angewandte Chemie - International Edition, 2021, 60, 1942-1950.	13.8	15
57	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie, 2020, 132, 17747-17752.	2.0	14
58	Ab initio studies of the oxidation of methane with oxo-metal cations. Chemical Physics Letters, 1997, 270, 357-362.	2.6	13
59	Nonadiabatic interactions between the ground and low-lying excited electronic states: Vibronic states of the Clâ€"HCl complex. Journal of Chemical Physics, 2001, 115, 5974-5983.	3.0	13
60	The stability of covalent dative bond significantly increases with increasing solvent polarity. Nature Communications, 2022, 13, 2107.	12.8	13
61	Photooxidation of Aniline Derivatives Can Be Activated by Freezing Their Aqueous Solutions. Environmental Science & Technology, 2017, 51, 13763-13770.	10.0	12
62	An Isolated Molecule of Iron(II) Phthalocyanin Exhibits Quintet Groundâ€State: A Nexus between Theory and Experiment. Chemistry - A European Journal, 2018, 24, 13413-13417.	3.3	12
63	Assigning the NH Stretches of the Guanine Tautomers Using Adiabatic Separation:â€‰ CCSD(T) Benchmark Calculations. Journal of Physical Chemistry A, 2008, 112, 1854-1856.	2.5	11
64	Interaction of acetonitrile with Na-zeolites: adsorption modes and vibrational dynamics in the zeolite channels and cavities. Physical Chemistry Chemical Physics, 2008, 10, 4189.	2.8	11
65	Biomolecule Analogues 2-Hydroxypyridine and 2-Pyridone Base Pairing on Ice Nanoparticles. Journal of Physical Chemistry A, 2016, 120, 4720-4730.	2.5	11
66	Ground state of the Fe(<scp>ii</scp>)-porphyrin model system corresponds to quintet: a DFT and DMRG-based tailored CC study. Physical Chemistry Chemical Physics, 2020, 22, 17033-17037.	2.8	11
67	Mechano-Optical Switching of a Single Molecule with Doublet Emission. ACS Nano, 2020, 14, 8931-8938.	14.6	11
68	Theoretical study of photoacidity of HCN: the effect of complexation with water. Physical Chemistry Chemical Physics, 2006, 8, 4866-4873.	2.8	10
69	Photodynamics of the adenine model 4-aminopyrimidine embedded within double strand of DNA. Collection of Czechoslovak Chemical Communications, 2011, 76, 631-643.	1.0	10
70	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorizationviavalence bond theory and high-level computational approaches. Physical Chemistry Chemical Physics, 2020, 22, 22003-22015.	2.8	10
71	Unexpected Photoreactivity in a NO₂-Functionalized Aluminum-MOF. Journal of Physical Chemistry C, 2015, 119, 26401-26408.	3.1	9
72	Spectroscopic Properties of Anisole at the Airâ€"Ice Interface: A Combined Experimentalâ€"Computational Approach. Langmuir, 2016, 32, 5755-5764.	3.5	9

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73	Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. Journal of Physical Chemistry A, 2020, 124, 10954-10966.	2.5	9
74	Structure-directed formation of the dative/covalent bonds in complexes with C₇₀â‹¯piperidine. Physical Chemistry Chemical Physics, 2021, 23, 4365-4375.	2.8	9
75	Structure and energetics of the anisoleâ€“Ar_n (n = 1, 2, 3) complexes: high-resolution resonant two-photon and threshold ionization experiments, and quantum chemical calculations. Physical Chemistry Chemical Physics, 2015, 17, 12530-12537.	2.8	8
76	Clustering of Uracil Molecules on Ice Nanoparticles. Journal of Physical Chemistry A, 2017, 121, 1069-1077.	2.5	8
77	Pathways to fluorescence via restriction of intramolecular motion in substituted tetraphenylethylenes. Physical Chemistry Chemical Physics, 2022, 24, 1722-1735.	2.8	8
78	Electronically Excited States of 1,4:5,8-Bismethano-1,4,4a,5,8,8a-hexahydronaphthalene, a Nonconjugated Diene:â€‰ Comparison of Theory and Experiment. Journal of the American Chemical Society, 1996, 118, 1235-1240.	13.7	7
79	Interaction of Lysine-Alanine-Alanine tripeptide with a fragment of DNA: An empirical potential study. Journal of Computational Chemistry, 1991, 12, 9-16.	3.3	6
80	Addition Reaction between Piperidine and C₆₀ to Form 1,4-Disubstituted C₆₀ Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study. Journal of the American Chemical Society, 2021, 143, 10930-10939.	13.7	6
81	First electronically excited state of the waterâ€“argon complex: an analytical fit to the CASPT2 potential. Chemical Physics Letters, 1999, 300, 561-568.	2.6	5
82	The effect of dimerization on the excited state behavior of methylated xanthine derivatives: a computational study. Photochemical and Photobiological Sciences, 2013, 12, 1496.	2.9	5
83	Spin Crossover in Iron(II) Porphyrazine Induced by Noncovalent Interactions Combined with Hybridization of Iron(II) Porphyrazine and Ligandâ€™s Orbitals: CASPT2, CCSD(T), and DFT Studies. Journal of Physical Chemistry C, 2019, 123, 23186-23194.	3.1	5
84	Reliability of DFT Methods for Description of Cu Sites and Their Interaction with NO in Zeolites. Collection of Czechoslovak Chemical Communications, 1998, 63, 1202-1212.	1.0	5
85	The Existence of a Nâ†’C Dative Bond in the C 60 â€“Piperidine Complex. Angewandte Chemie, 2021, 133, 1970-1978.	2.0	4
86	Binding Energies of the Ï€-Stacked Anisole Dimer: New Molecular Beam-Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6637-6637.	3.3	3
87	Non-covalent interactions in anisoleâ€“(CO₂)_n (n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2017, 19, 22749-22758.	2.8	3
88	The unusual stability of Hâ€bonded complexes in solvent caused by greater solvation energy of complex compared to those of isolated fragments. Journal of Computational Chemistry, 2023, 44, 329-333.	3.3	3