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	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
2	Pathways to fluorescence via restriction of intramolecular motion in substituted tetraphenylethylenes. Physical Chemistry Chemical Physics, 2022, 24, 1722-1735.	2.8	8
3	The stability of covalent dative bond significantly increases with increasing solvent polarity. Nature Communications, 2022, 13, 2107.	12.8	13
4	The Existence of a Nâ†'C Dative Bond in the C 60 â€"Piperidine Complex. Angewandte Chemie, 2021, 133, 1970-1978.	2.0	4
5	The Existence of a Nâ†'C Dative Bond in the C₆₀â€"Piperidine Complex. Angewandte Chemie - International Edition, 2021, 60, 1942-1950.	13.8	15
6	Unravelling the Open-Shell Character of Peripentacene on Au(111). Journal of Physical Chemistry Letters, 2021, 12, 330-336.	4.6	36
7	Structure-directed formation of the dative/covalent bonds in complexes with C₇₀â¯piperidine. Physical Chemistry Chemical Physics, 2021, 23, 4365-4375.	2.8	9
8	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	4.3	57
9	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
10	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
11	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
12	On-Surface Hydrogenation of Buckybowls: From Curved Aromatic Molecules to Planar Non-KekulÃ© Aromatic Hydrocarbons. ACS Nano, 2020, 14, 16735-16742.	14.6	15
13	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
14	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
15	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
16	Mechano-Optical Switching of a Single Molecule with Doublet Emission. ACS Nano, 2020, 14, 8931-8938.	14.6	11
17	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie, 2020, 132, 17747-17752.	2.0	14
18	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie - International Edition, 2020, 59, 17594-17599.	13.8	33

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19	Mechanisms of Orthogonal Photodecarbonylation Reactions of 3-Hydroxyflavone-Based Acidâ€“Base Forms. Journal of Organic Chemistry, 2020, 85, 3527-3537.	3.2	27
20	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
21	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
22	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
23	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
24	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
25	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
26	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. Nature Communications, 2018, 9, 2831.	12.8	68
27	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
28	Clustering of Uracil Molecules on Ice Nanoparticles. Journal of Physical Chemistry A, 2017, 121, 1069-1077.	2.5	8
29	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
30	Non-covalent interactions in anisoleâ€“(CO₂)_n (n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2017, 19, 22749-22758.	2.8	3
31	Photooxidation of Aniline Derivatives Can Be Activated by Freezing Their Aqueous Solutions. Environmental Science & Technology, 2017, 51, 13763-13770.	10.0	12
32	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. ACS Nano, 2017, 11, 12402-12410.	14.6	550
33	Spectroscopic Properties of Anisole at the Airâ€“Ice Interface: A Combined Experimentalâ€“Computational Approach. Langmuir, 2016, 32, 5755-5764.	3.5	9
34	Solvatochromic fluorene-linked nucleoside and DNA as color-changing fluorescent probes for sensing interactions. Chemical Science, 2016, 7, 5775-5785.	7.4	55
35	Biomolecule Analogues 2-Hydroxypyridine and 2-Pyridone Base Pairing on Ice Nanoparticles. Journal of Physical Chemistry A, 2016, 120, 4720-4730.	2.5	11
36	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

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37	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
38	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
39	Resonant Infrared Multiple Photon Dissociation Spectroscopy of Anionic Nucleotide Monophosphate Clusters. Journal of Physical Chemistry B, 2015, 119, 7894-7901.	2.6	25
40	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
41	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
42	Unexpected Photoreactivity in a NO₂-Functionalized Aluminum-MOF. Journal of Physical Chemistry C, 2015, 119, 26401-26408.	3.1	9
43	Photodissociation of aniline Nâ€"H bonds in clusters of different nature. Physical Chemistry Chemical Physics, 2015, 17, 25004-25013.	2.8	15
44	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
45	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. Topics in Current Chemistry, 2014, 356, 1-37.	4.0	20
46	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
47	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
48	Excited state dynamics of DNA bases. International Reviews in Physical Chemistry, 2013, 32, 308-342.	2.3	185
49	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
50	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
51	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
52	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145.	2.8	84
53	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255.	2.5	84
54	The decay mechanism of photoexcited guanine â˜' A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304.	3.0	70

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55	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
56	The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227.	3.3	73
57	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
58	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
59	Does Stacking Restrain the Photodynamics of Individual Nucleobases?. Journal of the American Chemical Society, 2010, 132, 8261-8263.	13.7	67
60	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
61	The effect of C5 substitution on the photochemistry of uracil. Physical Chemistry Chemical Physics, 2010, 12, 4924.	2.8	19
62	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
63	Photodynamics Simulations of Thymine: Relaxation into the First Excited Singlet State. Journal of Physical Chemistry A, 2009, 113, 12686-12693.	2.5	85
64	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
65	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
66	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
67	Electronic coupling in the excited electronic state of stacked DNA base homodimers. Physical Chemistry Chemical Physics, 2007, 9, 1672.	2.8	48
68	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
69	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
70	Theoretical study of photoacidity of HCN: the effect of complexation with water. Physical Chemistry Chemical Physics, 2006, 8, 4866-4873.	2.8	10
71	The vibrational dynamics of carbon monoxide in a confined spaceâ€”CO in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 4849-4852.	2.8	74
72	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

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73	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
74	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
75	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
76	On the Existence of CuI Pairs in ZSM-5â€”A Computational Study. Chemistry - A European Journal, 2002, 8, 2099.	3.3	33
77	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
78	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
79	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
80	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
81	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
82	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
83	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
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	Ab initio studies of the oxidation of methane with oxo-metal cations. Chemical Physics Letters, 1997, 270, 357-362.	2.6	13
86	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
87	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
88	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