Nadja Doslic

List of Publications by Year
in descending order

53	1,219	304743	395702
papers	citations	22 h-index	33 g-index

53	53	53	1412
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mixed-quantum-classical or fully-quantized dynamics? A unified code to compare methods. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200386.	3.4	11
2	A Computational Approach to Nontraditional Intrinsic Luminescence: Vibrationally Resolved Absorption and Fluorescence Spectra of DABCO. Journal of Physical Chemistry A, 2022, 126, 1094-1102.	2.5	0
3	Discrimination of Excited States of Acetylacetone through Theoretical Molecular-Frame Photoelectron Angular Distributions. Molecules, 2022, 27, 1811.	3.8	0
4	On the propensity of formation of cyclobutane dimers in face-to-face and face-to-back uracil stacks in solution. Physical Chemistry Chemical Physics, 2022, 24, 14836-14845.	2.8	1
5	Excited State Intramolecular Proton Transfer (ESIPT) from -NH₂ to the Carbon Atom of a Naphthyl Ring. Journal of Organic Chemistry, 2022, 87, 9148-9156.	3.2	1
6	Simulation of UV absorption spectra and relaxation dynamics of uracil and uracilâ€“water clusters. Physical Chemistry Chemical Physics, 2021, 23, 2594-2604.	2.8	17
7	Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pumpâ€“Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorwayâ€“Window Representation. Journal of Chemical Theory and Computation, 2021, 17, 2394-2408.	5.3	16
8	Combined Surface-Hopping, Dyson Orbital, and B-Spline Approach for the Computation of Time-Resolved Photoelectron Spectroscopy Signals: The Internal Conversion in Pyrazine. Journal of Chemical Theory and Computation, 2021, 17, 5098-5109.	5.3	11
9	Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. Journal of Physical Chemistry Letters, 2021, 12, 11736-11744.	4.6	9
10	Photoionization of pyrrole from the $$B_2$$ state: a computational study on the effects of Rydbergâ€“valence mixing. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
11	Toward Understanding Optical Properties of Amyloids: A Reaction Path and Nonadiabatic Dynamics Study. Journal of the American Chemical Society, 2020, 142, 18042-18049.	13.7	28
12	Photoelimination of Nitrogen from Diazoalkanes: Involvement of Higher Excited Singlet States in the Carbene Formation. Journal of the American Chemical Society, 2020, 142, 9718-9724.	13.7	4
13	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	3.0	44
14	Highly Efficient Algorithms for CIS Type Excited State Wave Function Overlaps. Journal of Chemical Theory and Computation, 2019, 15, 3461-3469.	5.3	26
15	UV absorption spectra of DNA bases in the 350â€“190 nm range: assignment and state specific analysis of solvation effects. Physical Chemistry Chemical Physics, 2019, 21, 22782-22793.	2.8	14
16	Acetylacetone photodynamics at a seeded free-electron laser. Nature Communications, 2018, 9, 63.	12.8	72
17	Comparative study of the photodynamics of malonaldehyde and acetylacetone. Chemical Physics, 2018, 515, 622-627.	1.9	3
18	Photochemistry of 1â€•and 2â€Naphthols and Their Water Clusters: The Role of ¹Ï€Ï€*(L_a) Mediated Hydrogen Transfer to Carbon Atoms. Chemistry - A European Journal, 2017, 23, 8244-8251.	3.3	18

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19	Substitution pattern on anthrol carbaldehydes: excited state intramolecular proton transfer (ESIPT) with a lack of phototautomer fluorescence. Physical Chemistry Chemical Physics, 2017, 19, 28439-28449.	2.8	6
20	Mechanism of ultrafast non-reactive deactivation of the retinal chromophore in non-polar solvents. Physical Chemistry Chemical Physics, 2017, 19, 25970-25978.	2.8	8
21	Nonradiative Relaxation Mechanisms of UV Excited Phenylalanine Residues: A Comparative Computational Study. Molecules, 2017, 22, 493.	3.8	11
22	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	3.0	20
23	Photochemical deactivation pathways of microsolvated hydroxylamine. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 328, 10-15.	3.9	4
24	How does tetraphenylethylene relax from its excited states?. Physical Chemistry Chemical Physics, 2016, 18, 11606-11609.	2.8	86
25	Timescales of Nâ€“H bond dissociation in pyrrole: a nonadiabatic dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 19012-19020.	2.8	40
26	Exploration of Excited State Deactivation Pathways of Adenine Monohydrates. Journal of Physical Chemistry A, 2015, 119, 10637-10644.	2.5	37
27	Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 2112-2124.	2.6	33
28	Non-radiative relaxation of UV photoexcited phenylalanine residues: probing the role of conical intersections by chemical substitution. Physical Chemistry Chemical Physics, 2014, 16, 2285.	2.8	28
29	Excited State Intramolecular Proton Transfer (ESIPT) from Phenol to Carbon in Selected Phenylnaphthols and Naphthylphenols. Journal of Organic Chemistry, 2013, 78, 1811-1823.	3.2	40
30	Unraveling the Mechanisms of Nonradiative Deactivation in Model Peptides Following Photoexcitation of a Phenylalanine Residue. Journal of the American Chemical Society, 2012, 134, 20340-20351.	13.7	66
31	Photoinduced Dynamics of Formic Acid Monomers and Dimers: The Role of the Double Hydrogen Bond. Journal of Physical Chemistry A, 2012, 116, 11467-11475.	2.5	26
32	One catalyst for both enantiomers: uncovering the inversion of enantioselectivity in cinchona-mediated desymmetrization of glutaric meso-anhydrides. Tetrahedron, 2012, 68, 8311-8317.	1.9	11
33	Very Efficient Generation of Quinone Methides through Excited State Intramolecular Proton Transfer to a Carbon Atom. Chemistry - A European Journal, 2012, 18, 10617-10623.	3.3	28
34	Fluxionality of Hydrogen Ligands in Fe(H)₂(H₂)(PEtPh₂)₃. Inorganic Chemistry, 2011, 50, 10740-10747.	4.0	15
35	Localization of the Counterion of the Protonated Schiff Base of n-butylretinal in Solution. Croatica Chemica Acta, 2011, 84, 221-231.	0.4	4
36	Quantum mechanical study of secondary structure formation in protected dipeptides. Physical Chemistry Chemical Physics, 2010, 12, 4678.	2.8	7

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37	Shaping the infrared spectrum of the acetic acid dimer in the OH-stretching range: Multiple conformers and anharmonic coupling. Chemical Physics Letters, 2009, 474, 248-252.	2.6	14
38	Generalized approximation to the reaction path: The formic acid dimer case. Journal of Chemical Physics, 2008, 128, 084103.	3.0	26
39	Ground and asymmetric CO-stretch excited state tunneling splittings in the formic acid dimer. Journal of Chemical Physics, 2007, 127, 014309.	3.0	26
40	Theoretical modeling of the formic acid dimer infrared spectrum: Shaping the Oâ€“H stretch band. Chemical Physics, 2007, 338, 121-126.	1.9	22
41	Terahertz-Laser Control of Large Amplitude Vibrational Motion in the Sub-One-Cycle Pulse Limit. Journal of Physical Chemistry A, 2006, 110, 12400-12405.	2.5	9
42	Anharmonic vibrational spectra of acetylacetone. International Journal of Quantum Chemistry, 2006, 106, 1367-1374.	2.0	16
43	Generalization of the Rabi population inversion dynamics in the sub-one-cycle pulse limit. Physical Review A, 2006, 74, .	2.5	33
44	Infrared Spectroscopy of the Intramolecular Hydrogen Bond in Acethylacetone: A Computational Approach. Journal of Physical Chemistry A, 2005, 109, 4185-4194.	2.5	51
45	Analytic pulse design for selective population transfer in many-level quantum systems: Maximizing the amplitude of population oscillations. Physical Review A, 2004, 70, .	2.5	7
46	Exploring the potential energy surface for proton transfer in acetylacetone. Chemical Physics, 2004, 306, 201-207.	1.9	31
47	Hydrogen bonding in malonaldehyde: a density functional and reparametrized semiempirical approach. Chemical Physics, 2003, 293, 41-52.	1.9	19
48	The Intramolecular Hydrogen-Bond in Malonaldehyde as Seen by Infrared Spectroscopy. A Four-Dimensional Model Study. Zeitschrift Fur Physikalische Chemie, 2003, 217, 1507-1524.	2.8	36
49	Proton transfer in malonaldehyde: a model three-dimensional study. Chemical Physics Letters, 2002, 358, 337-343.	2.6	36
50	Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy. Chemical Physics, 2000, 255, 247-257.	1.9	9
51	Ultrafast photoinduced dissipative hydrogen switching dynamics in thioacetylacetone. Physical Chemistry Chemical Physics, 1999, 1, 1249-1257.	2.8	63
52	The â€œHydrogen-Subwayâ€ Tunneling Approach to Intramolecular Hydrogen Transfer Reactions Controlled by Ultrashort Laser Pulses. Journal of Physical Chemistry A, 1998, 102, 9645-9650.	2.5	70
53	A new classical method for dynamical calculation in molecular systems. Molecular Physics, 1997, 90, 599-609.	1.7	5