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	How does tetraphenylethylene relax from its excited states?. Physical Chemistry Chemical Physics, 2016, 18, 11606-11609.	2.8	86
2	Acetylacetone photodynamics at a seeded free-electron laser. Nature Communications, 2018, 9, 63.	12.8	72
3	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
4	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
5	Ultrafast photoinduced dissipative hydrogen switching dynamics in thioacetylacetone. Physical Chemistry Chemical Physics, 1999, 1, 1249-1257.	2.8	63
6	Infrared Spectroscopy of the Intramolecular Hydrogen Bond in Acethylacetone: A Computational Approach. Journal of Physical Chemistry A, 2005, 109, 4185-4194.	2.5	51
7	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	3.0	44
8	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
9	Timescales of Nâ€“H bond dissociation in pyrrole: a nonadiabatic dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 19012-19020.	2.8	40
10	Exploration of Excited State Deactivation Pathways of Adenine Monohydrates. Journal of Physical Chemistry A, 2015, 119, 10637-10644.	2.5	37
11	Proton transfer in malonaldehyde: a model three-dimensional study. Chemical Physics Letters, 2002, 358, 337-343.	2.6	36
12	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
13	Generalization of the Rabi population inversion dynamics in the sub-one-cycle pulse limit. Physical Review A, 2006, 74, .	2.5	33
14	Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 2112-2124.	2.6	33
15	Exploring the potential energy surface for proton transfer in acetylacetone. Chemical Physics, 2004, 306, 201-207.	1.9	31
16	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
17	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
18	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

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19	Ground and asymmetric CO-stretch excited state tunneling splittings in the formic acid dimer. Journal of Chemical Physics, 2007, 127, 014309.	3.0	26
20	Generalized approximation to the reaction path: The formic acid dimer case. Journal of Chemical Physics, 2008, 128, 084103.	3.0	26
21	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
22	Highly Efficient Algorithms for CIS Type Excited State Wave Function Overlaps. Journal of Chemical Theory and Computation, 2019, 15, 3461-3469.	5.3	26
23	Theoretical modeling of the formic acid dimer infrared spectrum: Shaping the Oâ€“H stretch band. Chemical Physics, 2007, 338, 121-126.	1.9	22
24	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	3.0	20
25	Hydrogen bonding in malonaldehyde: a density functional and reparametrized semiempirical approach. Chemical Physics, 2003, 293, 41-52.	1.9	19
26	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
27	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
28	Anharmonic vibrational spectra of acetylacetone. International Journal of Quantum Chemistry, 2006, 106, 1367-1374.	2.0	16
29	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
30	Fluxionality of Hydrogen Ligands in Fe(H)₂(H₂)(PEtPh₂)₃. Inorganic Chemistry, 2011, 50, 10740-10747.	4.0	15
31	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
32	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
33	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
34	Nonradiative Relaxation Mechanisms of UV Excited Phenylalanine Residues: A Comparative Computational Study. Molecules, 2017, 22, 493.	3.8	11
35	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
36	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

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37	Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy. Chemical Physics, 2000, 255, 247-257.	1.9	9
38	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
39	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
40	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
41	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
42	Quantum mechanical study of secondary structure formation in protected dipeptides. Physical Chemistry Chemical Physics, 2010, 12, 4678.	2.8	7
43	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
44	A new classical method for dynamical calculation in molecular systems. Molecular Physics, 1997, 90, 599-609.	1.7	5
45	Localization of the Counterion of the Protonated Schiff Base of n-butylretinal in Solution. Croatica Chemica Acta, 2011, 84, 221-231.	0.4	4
46	Photochemical deactivation pathways of microsolvated hydroxylamine. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 328, 10-15.	3.9	4
47	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
48	Comparative study of the photodynamics of malonaldehyde and acetylacetone. Chemical Physics, 2018, 515, 622-627.	1.9	3
49	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
50	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
51	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
52	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
53	Discrimination of Excited States of Acetylacetone through Theoretical Molecular-Frame Photoelectron Angular Distributions. Molecules, 2022, 27, 1811.	3.8	0