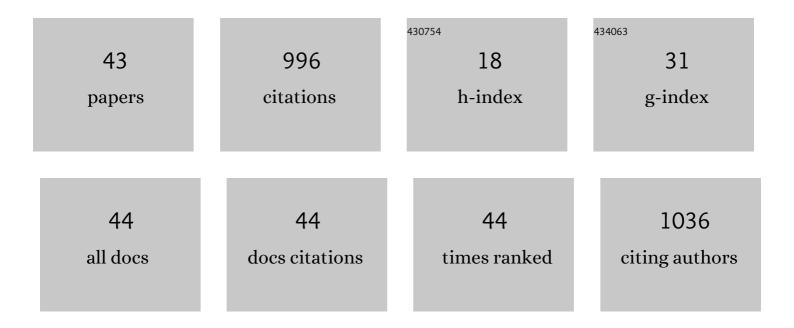
MichaÅ, F Rode

List of Publications by Year in descending order

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MICHAL FRODE

#	Article	IF	CITATIONS
1	Effect of Chemical Substituents on the Energetical Landscape of a Molecular Photoswitch: An Ab Initio Study. Journal of Physical Chemistry A, 2010, 114, 11879-11889.	1.1	86
2	Ab initio study of the O2 binding in dicopper complexes. Theoretical Chemistry Accounts, 2005, 114, 309-317.	0.5	76
3	A Computational Study on the Mechanism of Intramolecular Oxoâ^Hydroxy Phototautomerism Driven by Repulsive ï∈ïƒ* State. Journal of Physical Chemistry A, 2008, 112, 13655-13661.	1.1	70
4	The importance of high-order correlation effects for the CO–CO interaction potential. Chemical Physics Letters, 1999, 314, 326-332.	1.2	60
5	A Bistable Molecular Switch Driven by Photoinduced Hydrogenâ€Atom Transfer. ChemPhysChem, 2009, 10, 2290-2295.	1.0	53
6	Suppression of Angular Forces in Collisions of Non-S-State Transition Metal Atoms. Physical Review Letters, 2005, 94, 013202.	2.9	51
7	Switching the Conductance of a Single Molecule by Photoinduced Hydrogen Transfer. Journal of Physical Chemistry C, 2009, 113, 10315-10318.	1.5	51
8	Excitedâ€ 5 tate Intramolecular Proton Transfer: Photoswitching in Salicylidene Methylamine Derivatives. ChemPhysChem, 2014, 15, 1643-1652.	1.0	49
9	Photophysics of Schiff Bases: Theoretical Study of Salicylidene Methylamine. ChemPhysChem, 2012, 13, 4287-4294.	1.0	45
10	Photophysics of inter- and intra-molecularly hydrogen-bonded systems: Computational studies on the pyrrole–pyridine complex and 2(2′-pyridyl)pyrrole. Chemical Physics, 2008, 347, 413-421.	0.9	40
11	Computational Study on the Photophysics of Protonated Benzene. Journal of Physical Chemistry A, 2009, 113, 5865-5873.	1.1	38
12	7-Hydroxyquinoline-8-carbaldehydes. 1. Ground- and Excited-State Long-Range Prototropic Tautomerization. Journal of Physical Chemistry A, 2013, 117, 9127-9146.	1.1	31
13	Ultrafast dynamics of the ESIPT photoswitch <i>N</i> -(3-pyridinyl)-2-pyridinecarboxamide. Physical Chemistry Chemical Physics, 2018, 20, 2646-2655.	1.3	29
14	Excited state intramolecular proton transfer in hydroxyanthraquinones: Toward predicting fading of organic red colorants in art. Science Advances, 2019, 5, eaaw5227.	4.7	26
15	Photophysical properties of betaxanthins: miraxanthinÂV – insight into the excited-state deactivation mechanism from experiment and computations. RSC Advances, 2017, 7, 6411-6421.	1.7	23
16	Reply to the Comment on "The importance of high-order correlation effects for the CO–CO interaction potential―[Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 424-425.	1.2	22
17	Interactions of transition metal atoms with He. European Physical Journal D, 2004, 31, 429-437.	0.6	21
18	Effect of chemical substitutions on photo-switching properties of 3-hydroxy-picolinic acid studied by <i>ab initio</i> methods. Journal of Chemical Physics, 2014, 140, 084301.	1.2	19

MichaÅ, F Rode

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19	Photochromic reaction in 3 <i>H</i> -naphthopyrans studied by vibrational spectroscopy and quantum chemical calculations. Physical Chemistry Chemical Physics, 2019, 21, 11861-11870.	1.3	17
20	Control of the Photo-Isomerization Mechanism in 3H-Naphthopyrans to Prevent Formation of Unwanted Long-Lived Photoproducts. International Journal of Molecular Sciences, 2020, 21, 7825.	1.8	16
21	Ab initio study on the excited state proton transfer mediated photophysics of 3-hydroxy-picolinic acid. Chemical Physics, 2012, 409, 41-48.	0.9	15
22	Electronic Spectra and Reversible Photoisomerization of Protonated Naphthalenes in Solid Neon. Journal of Physical Chemistry A, 2013, 117, 351-360.	1.1	15
23	The (H2O)2CO ternary complex: cyclic or linear?. Chemical Physics Letters, 2001, 342, 220-230.	1.2	14
24	Photophysics of indole-2-carboxylic acid in an aqueous environment studied by fluorescence spectroscopy in combination with ab initio calculations. Physical Chemistry Chemical Physics, 2012, 14, 2078.	1.3	12
25	Direct Arylation of Dipyrrolonaphthyridinediones Leads to Redâ€Emitting Dyes with Conformational Freedom. Chemistry - A European Journal, 2018, 24, 855-864.	1.7	12
26	Ultrafast Dynamics of the Transoidâ€ <i>cis</i> Isomer Formed in Photochromic Reaction from 3 <i>H</i> â€Naphthopyran. ChemPhysChem, 2020, 21, 1402-1407.	1.0	12
27	7-Hydroxyquinoline-8-carbaldehydes. 2. Prototropic Equilibria. Journal of Physical Chemistry A, 2013, 117, 9147-9155.	1.1	11
28	Ab initio calculations of nonadditive effects in the trimers (H2O)2â<¯XY,XY=N2, BF, CS. Chemical Physics Letters, 2002, 358, 237-249.	1.2	10
29	The nonadditive effects in the mixed trimers composed of the water dimer and diatomics H2, HF, HCl, HBr, and ClF. Chemical Physics Letters, 2003, 368, 754-768.	1.2	9
30	Photochemistry of the water dimer: Time-dependent quantum wave-packet description of the dynamics at the S1-S0 conical intersection. Journal of Chemical Physics, 2009, 131, 134307.	1.2	9
31	Structure – chiroptical properties relationship of cisoid enones with an α-methylenecyclopentanone unit. RSC Advances, 2014, 4, 43977-43993.	1.7	9
32	Synthesis, photophysics and excited state structure of 1,8-di(p-tolyl)-1,3,5,7-octatetrayne. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 217, 299-307.	2.0	7
33	Multipeak negative differential resistance from interplay between nonlinear stark effect and double-branch current flow. RSC Advances, 2014, 4, 52933-52939.	1.7	7
34	Ferroelectric molecular field-switch based on double proton transfer process: Static and dynamical simulations. Journal of Chemical Physics, 2016, 144, 134303.	1.2	7
35	Cisoid-cis intermediate plays a crucial role in decolouration rate in photochromic reaction of 8H-pyranoquinazolines and 3H-naphthopyrans. Dyes and Pigments, 2022, 201, 110249.	2.0	6
36	Mechanistic insights into photochromic 3H-naphthopyran showing strong photocoloration. Scientific Reports, 2022, 12, .	1.6	6

MichaÅ, F Rode

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37	The effect of electron detachment on the structure and properties of the chlorine-acetonitrile anionic complex. Journal of Chemical Physics, 2004, 121, 6277-6281.	1.2	3
38	Photochemical and thermal isomerizations of C2h and C2v forms of para-benzoquinone dioxime: A matrix-isolation study. Journal of Molecular Structure, 2010, 976, 181-189.	1.8	3
39	Contacts for organic switches with carbon-nanotube leads. Nanotechnology, 2015, 26, 245201.	1.3	3
40	Structural studies on the stereoisomerism of a natural dye miraxanthin I. New Journal of Chemistry, 2019, 43, 18165-18174.	1.4	2
41	Ultrafast Dynamics of a Bistable Intramolecular Proton Transfer Switch. Springer Proceedings in Physics, 2015, , 399-402.	0.1	1
42	Publisher's Note: Suppression of Angular Forces in Collisions of Non-S-State Transition Metal Atoms [Phys. Rev. Lett.94, 013202 (2005)]. Physical Review Letters, 2005, 94, .	2.9	0
43	Ultrafast Dynamics of a Bistable Intramolecular Proton Transfer Switch. , 2014, , .		0