Marcin Andrzejak

List of Publications by Year
in descending order

47	876	516710 16	501196 28
papers	citations	h-index	g-index

48	48	48	679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 28970-28981.	2.8	114
2	A uniform approach to the description of multicenter bonding. Physical Chemistry Chemical Physics, 2014, 16, 20514-20523.	2.8	112
3	The role of the longâ€•range exchange corrections in the description of electron delocalization in aromatic species. Journal of Computational Chemistry, 2017, 38, 1640-1654.	3.3	69
4	Theoretical calculation of the electro-absorption spectrum of the Î±-sexithiophene single crystal. Journal of Chemical Physics, 2002, 117, 1328-1335.	3.0	37
5	Quantum chemical results as input for solid state calculations: charge transfer states in molecular crystals. Computational and Theoretical Chemistry, 2000, 527, 91-102.	1.5	36
6	Aromaticity of acenes: the model of migrating Ï€-circuits. Physical Chemistry Chemical Physics, 2018, 20, 13430-13436.	2.8	36
7	Vibronic interpretation of the low-energy absorption spectrum of the sexithiophene single crystal. Journal of Chemical Physics, 2000, 113, 11306-11314.	3.0	34
8	The structure of the boron trifluoride-ammonia complex: a Fourier transform matrix isolation infrared spectroscopic and ab initio molecular orbital study. Vibrational Spectroscopy, 1996, 12, 221-235.	2.2	33
9	Avoiding pitfalls of a theoretical approach: the harmonic oscillator measure of aromaticity index from quantum chemistry calculations. Structural Chemistry, 2013, 24, 1171-1184.	2.0	31
10	The Vibrational Spectra of the Boron Halides and Their Molecular Complexes. 3.Ab InitioPredictions of the Structures, Energetics, and Mulliken Atomic Charges of the Complexes of Boron Trifluoride with Some Linear Nitrogen Donors. Journal of Chemical Information and Computer Sciences, 1996, 36, 377-384.	2.8	29
11	Vibronic coupling in dimer â€“ A convenient approximation revisited. Chemical Physics, 2007, 335, 155-163.	1.9	27
12	Vibronic Effects in the 1¹B_u(1¹B₂) Excited Singlet States of Oligothiophenes. Fluorescence Study of the 1¹A_g(1¹A₁) â†• 1¹B_u(1¹B₂) Transition in Terms of DFT, TDDFT, and CASSCF Methods. Journal of Physical Chemistry A, 2008, 112, 13737-13744.	2.5	21
13	The vibrational spectra of the boron halides and their molecular complexes: Part 7. Ab initio predictions of the infrared spectra of the complexes of boron trifluoride with some linear nitrogen donors. Journal of Molecular Structure, 1999, 509, 287-295.	3.6	20
14	Fourier Transform Infrared and Raman and Surface-Enhanced Raman Spectroscopy Studies of a Novel Group of Boron Analogues of Aminophosphonic Acids. Journal of Physical Chemistry A, 2012, 116, 10004-10014.	2.5	19
15	The elusive excited states of bithiophene: a CASPT2 detective story. Theoretical Chemistry Accounts, 2011, 129, 161-172.	1.4	18
16	Vibrational characterization of <scp>L</scp>â€valine phosphonate dipeptides: FTâ€IR, FTâ€RS, and SERS spectroscopy studies and DFT calculations. Journal of Raman Spectroscopy, 2011, 42, 958-979.	2.5	17
17	Polarization energy calculations of charge transfer states in the Î±-sexithiophene crystal. Synthetic Metals, 2000, 109, 97-100.	3.9	16
18	The lowest triplet states of bridged cis-2,2â€²-bithiophenes â€“ theory vs. experiment. Physical Chemistry Chemical Physics, 2015, 17, 5328-5337.	2.8	16

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19	Calculation of refractive indices and local electric field tensors in Î±-sexithiophene crystal. Chemical Physics Letters, 2001, 336, 357-363.	2.6	15
20	Davydov splitting in the sexithiophene crystal. Chemical Physics Letters, 2001, 343, 139-142.	2.6	15
21	Absorption and magnetic circular dichroism (MCD) studies of 1,4,5,8-naphthalenetetracarboxy diimides in terms of CASSCF method and FC theory. Chemical Physics, 2004, 300, 93-105.	1.9	14
22	Photophysical properties of some donorâ€“acceptor 1H-pyrazolo[3,4-b]quinolines. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 187, 78-86.	3.9	14
23	From Saturated BN Compounds to Isoelectronic BN/CC Counterparts: An Insight from Computational Perspective. Chemistry - A European Journal, 2015, 21, 15299-15307.	3.3	14
24	Is Vibrational Coherence a Byproduct of Singlet Exciton Fission?. Journal of Physical Chemistry C, 2019, 123, 91-101.	3.1	13
25	Comparison of adsorption mechanism on colloidal silver surface of alafosfalin and its analogs. Journal of Raman Spectroscopy, 2008, 39, 1238-1249.	2.5	11
26	Joint theoretical and experimental study on the phosphorescence of 2,2â€²-bithiophene. Physical Chemistry Chemical Physics, 2014, 16, 5605.	2.8	10
27	Quantitatively Adequate Calculations of the H-Chelate Ring Distortion upon the S₀ â†' S₁(Ï€Ï€*) Excitation in Internally H-Bonded o-Anthranilic Acid: CC2 Coupled-Cluster versus TDDFT. Journal of Physical Chemistry A, 2018, 122, 6243-6255.	2.5	10
28	Vibronic relaxation energies of acene-related molecules upon excitation or ionization. Physical Chemistry Chemical Physics, 2018, 20, 14061-14071.	2.8	9
29	Temperature dependence of fullerene electroabsorption spectra â€“ model calculations. Chemical Physics, 1999, 243, 149-157.	1.9	7
30	Mesoscopic disorder in thin film spectra: absorption spectroscopy of sexithiophene. Chemical Physics Letters, 2000, 332, 435-441.	2.6	7
31	The circular dichroism (CD) studies of bis-1,8-naphthalimide. The theoretical analysis in terms of density functional and vibronic dimer theories. Chemical Physics Letters, 2010, 496, 74-79.	2.6	6
32	Evolution of physical properties of conjugated systems. Physica Status Solidi (B): Basic Research, 2012, 249, 306-316.	1.5	6
33	Theoretical Modeling of Deuteration-Induced Shifts of the 0â€“0 Bands in Absorption Spectra of Selected Aromatic Amines: The Role of the Double-Well Potential. Journal of Physical Chemistry A, 2013, 117, 12770-12782.	2.5	6
34	The electronic absorption study of imide anion radicals in terms of time dependent density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2029-2032.	3.9	5
35	LIF excitation spectra for S0â†'S1 transition of deuterated anthranilic acid COOD, ND2 in supersonic-jet expansion. Journal of Molecular Spectroscopy, 2010, 264, 129-136.	1.2	5
36	Theoretical Estimates of Charge Transfer State Energies in Sexithiophene. Molecular Crystals and Liquid Crystals, 2001, 355, 65-75.	0.3	4

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37	SPECTRAL EFFECTS OF MICROSCOPIC AND MESOSCOPIC DISORDER IN ORGANIC FILMS â€" MODEL CALCULATIONS. International Journal of Modern Physics B, 2001, 15, 3651-3655.	2.0	4
38	Consistent Franckâ€"Condon modeling of geometry changes for the S0â†'S1(Ï€Ï€*) excitation in anthranilic acid: LIF spectroscopy aided by CC2 or TDDFT vibrations. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 242, 106747.	2.3	3
39	The magnetic circular dichroism (MCD) and absorption studies of 1,8-naphthalimide. The theoretical analysis in terms of density functional (DF) and coupled cluster (CC) theories. Chemical Physics Letters, 2013, 555, 87-91.	2.6	2
40	Isotopic effects in the S1 exited state of anthranilic acid deuterated in various positions in substituent groups. Supersonic-jet LIF spectroscopy and CC2 ab initio study. Chemical Physics, 2015, 450-451, 46-58.	1.9	2
41	Vibrational and ab initio molecular dynamics studies of bradykinin. Journal of Molecular Structure, 2016, 1116, 272-278.	3.6	2
42	Soft Selection Rules for Femtosecond Pumpâ€"Probe Vibrational Coherence Spectroscopy. Journal of Physical Chemistry C, 2020, 124, 23501-23510.	3.1	2
43	Limitations of Generic Chromophore Concept for Femtosecond Vibrational Coherences. Journal of Physical Chemistry C, 2020, 124, 3529-3535.	3.1	2
44	Excited states manifold of 2,2â€²-bithiophene: basis set dependence study. Molecular Physics, 2017, 115, 2823-2832.	1.7	1
45	Vibrational Spectroscopy of Linear Carbon Chains. , 2011, , 375-415.		1
46	SPECTRAL EFFECTS OF MICROSCOPIC AND MESOSCOPIC DISORDER IN ORGANIC FILMS â€" MODEL CALCULATIONS. , 2001, , .		0
47	Optical Spectra of Oligofurans: A Theoretical Approach to the Transition Energies, Reorganization Energies, and the Vibronic Activity. Molecules, 2021, 26, 7163.	3.8	0