Mateusz Zbigniew Brela

List of Publications by Year
in descending order

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36 papers	479 citations	759055 12 h-index	713332 21 g-index
38 all docs	38 docs citations	38 times ranked	633 citing authors

#	Article	IF	Citations
1	Near-Infrared fluorescent unsymmetrical aza-BODIPYs: Synthesis, photophysics and TD-DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 271, 120898.	2.0	3
2	Influence of Hydrogen Bonds and Ï€â€“Ï€ Interactions on the Fluorescence of Crystalline (N-Alkylpyridyl)enamino-pyrrolo[2,3-b]quinoxalin-2-one Derivatives. Crystal Growth and Design, 2022, 22, 1571-1582.	1.4	2
3	Unravelling the nature of a tolueneâ€“fumaronitrile complex. Physical Chemistry Chemical Physics, 2021, 23, 16128-16141.	1.3	2
4	Displacive or Order-Disorder Phase Transition? The H-bond Dynamics in Multicaloric Ammonium Sulfate. Acta Materialia, 2021, 209, 116782.	3.8	9
5	The origin of conformational solvatochromism in phenylmethylidene-bis(pyrrolo[2,3-b]quinoxaline) derivative. Dyes and Pigments, 2021, 193, 109475.	2.0	0
6	Chasing the Co-crystal Disappearing Polymorph with Ab Initio Methods. Crystal Growth and Design, 2021, 21, 6902-6912.	1.4	3
7	A comparison of the hydrogen bond interaction dynamics in the adenine and thymine crystals: BOMD and spectroscopic study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 237, 118398.	2.0	4
8	Quantum-mechanical study of energies, structures and vibrational spectra of the HF complexed with dimethyl ether. Chemical Physics Letters, 2019, 731, 136590.	1.2	2
9	Comparison of the Hydrogen Bond Interaction Dynamics in the Guanine and Cytosine Crystals: Ab Initio Molecular Dynamics and Spectroscopic Study. Journal of Physical Chemistry A, 2019, 123, 10757-10763.	1.1	8
10	The synthesis and characterization of tetramic acid derivatives as Mdm2-p53 inhibitors. Journal of Molecular Structure, 2019, 1189, 161-174.	1.8	2
11	Path Integral Calculation of the Hydrogen/Deuterium Kinetic Isotope Effect in Monoamine Oxidase A-Catalyzed Decomposition of Benzylamine. Molecules, 2019, 24, 4359.	1.7	10
12	Study of hydrogen bond dynamics in Nylon 6 crystals using IR spectroscopy and molecular dynamics focusing on the differences between Î± and Î³ crystal forms. International Journal of Quantum Chemistry, 2018, 118, e25595.	1.0	11
13	Spectroscopic study of uracil, 1-methyluracil and 1-methyl-4-thiouracil: Hydrogen bond interactions in crystals and ab-initio molecular dynamics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 194-201.	2.0	6
14	ETS-NOCV decomposition of the reaction force for double-proton transfer in formamide-derived systems. Journal of Molecular Modeling, 2018, 24, 27.	0.8	7
15	Molecular Dynamics Simulations of Vibrational Spectra of Hydrogen-Bonded Systems. , 2018, , 353-376.		2
16	Understanding the Structure of the Hydrogen Bond Network and Its Influence on Vibrational Spectra in a Prototypical Aprotic Ionic Liquid. Journal of Physical Chemistry B, 2018, 122, 9527-9537.	1.2	25
17	Proton dynamics in crystalline tropolone studied by Born-Oppenheimer molecular simulations. Chemical Physics Letters, 2018, 707, 54-60.	1.2	6
18	The Born-Oppenheimer molecular simulations of infrared spectra of crystalline poly-(R)-3-hydroxybutyrate with analysis of weak C Hâ‹¯O C hydrogen bonds. Chemical Physics Letters, 2017, 678, 112-118.	1.2	11

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19	Anion conducting methylated aliphatic <scp>PBI</scp> and its calculated properties. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 256-265.	2.4	11
20	Synthesis, crystal structures, and optical properties of the Ï€-Ï€ interacting pyrrolo[2,3-b]quinoxaline derivatives containing 2-thienyl substituent. Journal of Molecular Structure, 2017, 1146, 337-346.	1.8	37
21	Infrared Spectroscopy and Bornâ€“Oppenheimer Molecular Dynamics Simulation Study on Deuterium Substitution in the Crystalline Benzoic Acid. Journal of Physical Chemistry B, 2017, 121, 479-489.	1.2	9
22	The influence of the metal cations and microhydration on the reaction trajectory of the N3 â†" O2 thymine proton transfer: Quantum mechanical study. Journal of Computational Chemistry, 2017, 38, 2680-2692.	1.5	4
23	ETSâ€NOCV Decomposition of the Reaction Force: The HCN/CNH Isomerization Reaction Assisted by Water. Journal of Computational Chemistry, 2017, 38, 2076-2087.	1.5	19
24	Ammonium sulfate phase transition studied by ab initio calculations. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C956-C956.	0.0	0
25	Bornâ€“Oppenheimer Molecular Dynamics Study on Proton Dynamics of Strong Hydrogen Bonds in Aspirin Crystals, with Emphasis on Differences between Two Crystal Forms. Journal of Physical Chemistry B, 2016, 120, 3854-3862.	1.2	24
26	Explicit Solvent Modeling of IR and UVâ€“Vis Spectra of 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid. Journal of Physical Chemistry B, 2016, 120, 11026-11034.	1.2	12
27	Polymorphism driven optical properties of an anil dye. CrystEngComm, 2016, 18, 7249-7259.	1.3	29
28	Fluorescence excitation spectra of all-trans-1,6-diphenylhexatriene conformers: Adiabatic conformer equilibration in the 21Ag state. Chemical Physics Letters, 2016, 648, 19-24.	1.2	4
29	Phase Separated Methylated Polybenzimidazole (Oâ€PBI) Based Anion Exchange Membranes. Macromolecular Materials and Engineering, 2015, 300, 497-509.	1.7	13
30	Carâ€“Parrinello Molecular Dynamics Simulations of Infrared Spectra of Crystalline Vitamin C with Analysis of Double Minimum Proton Potentials for Medium-Strong Hydrogen Bonds. Journal of Physical Chemistry B, 2015, 119, 7922-7930.	1.2	20
31	Tetrazole substituted polymers for high temperature polymer electrolyte fuel cells. Journal of Materials Chemistry A, 2015, 3, 14389-14400.	5.2	28
32	Anion conducting polymers based on ether linked polybenzimidazole (PBI-OO). International Journal of Hydrogen Energy, 2014, 39, 2842-2853.	3.8	55
33	Analysis of the Bonding between Two M(Î¼-NAr[#]) Monomers in the Dimeric Metal(II) Imido Complexes {M(Î¼-NAr[#])}₂ [M = Si, Ge, Sn, Pb; Ar[#] = C₆H₃-2,6-(C₆H₂-2,4,6-R₃)₂]. The Stabilizing Role Played by R = Me and iPr. Inorganic Chemistry, 2014, 53, 2325-2332.	1.9	9
34	Experimental and theoretical investigations of the NiII complex with N-phosphorylated thiourea iPrNHC(S)NHP(O)(OPh)2. CrystEngComm, 2013, 15, 7845.	1.3	16
35	Carâ€“Parrinello simulation of the vibrational spectra of strong hydrogen bonds with isotopic substitution effects: Application to oxalic acid dihydrate. Chemical Physics Letters, 2013, 558, 88-92.	1.2	20
36	Carâ€“Parrinello Simulation of the Vibrational Spectrum of a Medium Strong Hydrogen Bond by Two-Dimensional Quantization of the Nuclear Motion: Application to 2-Hydroxy-5-nitrobenzamide. Journal of Physical Chemistry B, 2012, 116, 4510-4518.	1.2	55