Pawel Rodziewicz

List of Publications by Year
in descending order

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39 papers	692 citations	567144 15 h-index	580701 25 g-index
40 all docs	40 docs citations	40 times ranked	683 citing authors

#	Article	IF	Citations
1	Unusual spectroscopic properties of CF3H dissolved in liquified Ar, N2, CO, and CO2. Chemical Physics Letters, 2002, 352, 301-310.	1.2	69
2	Blue shifted F3CHâ‹¯FCD3 and Cl3CHâ‹¯FCD3 weakly H-bound complexes. Cryospectroscopic and ab initio study. Chemical Physics, 2005, 313, 225-243.	0.9	59
3	Ab Initio Studies of Electron Acceptor-Donor Interactions with Blue- and Red-Shifted Hydrogen Bonds. ChemPhysChem, 2005, 6, 1282-1292.	1.0	59
4	Formamide Dimers:â€‰ A Computational and Matrix Isolation Study. Journal of Physical Chemistry A, 2007, 111, 10552-10561.	1.1	59
5	Ab Initio Molecular Dynamics Freeâ€Energy Study of Microhydration Effects on the Neutralâ€“Zwitterion Equilibrium of Phenylalanine. ChemPhysChem, 2007, 8, 1959-1968.	1.0	35
6	Intramolecular Hydrogen Bonds in Lowâ€Molecularâ€Weight Polyethylene Glycol. ChemPhysChem, 2016, 17, 1143-1153.	1.0	31
7	Comparative studies of blue shifting and red shifting effects in fluoroform and acetylene cryogenic solutions. Journal of Molecular Structure, 2004, 705, 49-61.	1.8	29
8	Infrared spectra and relative stability of the F3CH/NH3 H-bonded complex in liquefied Xe. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1595-1602.	2.0	24
9	Solvent effect on the blue shifted weakly H-bound F3 CHâ€¦FCD3 complex. Journal of Molecular Structure, 2008, 880, 64-68.	1.8	24
10	Formic Acid Dimerization: Evidence for Species Diversity from First Principles Simulations. Journal of Physical Chemistry A, 2009, 113, 6266-6274.	1.1	23
11	Photocatalytic degradation of hazardous Food Yellow 13 in TiO2 and ZnO aqueous and river water suspensions. Catalysis Today, 2016, 266, 72-81.	2.2	22
12	Infrared studies of acetylene dissolved in liquefied Ar, Kr, N2, CO, and CO2. Journal of Molecular Structure, 2002, 614, 305-313.	1.8	18
13	Solvation of diclofenac in water from atomistic molecular dynamics simulations â€“ interplay between soluteâ€“solute and soluteâ€“solvent interactions. Physical Chemistry Chemical Physics, 2018, 20, 8629-8639.	1.3	18
14	Structural, Vibrational and Electronic Properties of Defective Singleâ€Walled Carbon Nanotubes Functionalised with Carboxyl Groups: Theoretical Studies. ChemPhysChem, 2015, 16, 2775-2782.	1.0	16
15	Structural stability of diclofenac vs. inhibition activity from ab initio molecular dynamics simulations. Comparative study with ibuprofen and ketoprofen. Structural Chemistry, 2017, 28, 999-1008.	1.0	16
16	A Domino Annulation Reaction under Willgerodtâ€“Kindler Conditions. Journal of Organic Chemistry, 2008, 73, 4644-4649.	1.7	15
17	Car-Parrinello Molecular Dynamics Study of a Blue-Shifted Intermolecular Weak-Hydrogen-Bond System. ChemPhysChem, 2005, 6, 1719-1724.	1.0	14
18	Structural flexibility of 4,4â€²-methylene diphenyl diisocyanate (4,4â€²-MDI): evidence from first principles calculations. Journal of Molecular Modeling, 2014, 20, 2097.	0.8	14

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19	Triple helical collagen-like peptide interactions with selected polyphenolic compounds. RSC Advances, 2015, 5, 95443-95453.	1.7	14
20	Noncovalent functionalization of single-walled carbon nanotubes by aromatic diisocyanate molecules: A computational study. Chemical Physics Letters, 2014, 598, 10-16.	1.2	13
21	Carâ€“Parrinello Molecular Dynamics Study of the Blue-Shifted F3CHâ‹…â‹…â‹…FCD3 System in Liquid N2. ChemPhysChem, 2006, 7, 1221-1228.	1.0	12
22	First-principles study of fluoroform adsorption on a hexagonal ice (0001) surface: weak hydrogen bondsâ€”strong structural effects. Physical Chemistry Chemical Physics, 2011, 13, 14101.	1.3	12
23	Ab initio study of NMR shielding of alkali earth metal ions in water complexes and magnetic moments of alkali earth metal nuclei. Chemical Physics Letters, 2013, 588, 57-62.	1.2	11
24	Theoretical study of Hal3CH/F2CD2 (Hal=F,Cl) and F3CH/FH heterodimers with blue shifted hydrogen bonds. Chemical Physics, 2006, 327, 193-201.	0.9	10
25	Cooperative effects in blue-shifted hydrogen bonded cluster of from first principles simulations. Chemical Physics, 2009, 361, 129-136.	0.9	10
26	Interplay between moleculeâ€“molecule and moleculeâ€“substrate interactions: first-principles study of fluoroform aggregates on a hexagonal ice (0001) surface. Physical Chemistry Chemical Physics, 2014, 16, 940-954.	1.3	10
27	Structural flexibility of the sulfur mustard molecule at finite temperature from Carâ€“Parrinello molecular dynamics simulations. Journal of Hazardous Materials, 2016, 306, 269-277.	6.5	10
28	Degeneracy Lifting Effect in the FTIR Spectrum of Fluoroform Trapped in a Nitrogen Matrix. An Experimental and Carâ€“Parrinello Molecular Dynamics Study. Journal of Physical Chemistry A, 2016, 120, 3497-3503.	1.1	7
29	CHâ‹¯B interactions in acetylene containing solutions: experimental and theoretical DFT studies. Journal of Molecular Structure, 2003, 645, 295-302.	1.8	6
30	Bis(2,2â€²:6â€²,2â€²â€²-terpyridine)ruthenium(II) bis(perchlorate) hemihydrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, m1414-m1415.	0.2	6
31	Adsorption of sulfur mustard on clean and water-saturated ZnO(10<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 277 Td (x calculations. Journal of Hazardous Materials, 2021, 402, 123503.	6.5	5
32	Covalent functionalization of single-walled carbon nanotubes through attachment of aromatic diisocyanate molecules from first principles. Chemical Physics Letters, 2015, 619, 103-108.	1.2	4
33	Impact of vacancy defects in single-walled carbon nanotube on the structural properties of covalently attached aromatic diisocyanates. Applied Surface Science, 2016, 362, 1-10.	3.1	4
34	Conformational diversity of the THF molecule in N2 matrix by means of FTIR matrix isolation experiment and Car-Parrinello molecular dynamics simulations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 238, 118425.	2.0	4
35	Experimental (Raman and IR) and computational (DFT, MP2) studies of conformational diversity of 1-chloromethyl-1-fluorosilacyclohexane. Journal of Molecular Structure, 2020, 1221, 128786.	1.8	4
36	Single-walled carbon nanotubes in tetrahydrofuran solution: microsolvation from first-principles calculations. Journal of Molecular Modeling, 2019, 25, 206.	0.8	3

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37	A computational study of intramolecular hydrogen bonds breaking/formation: impact on the structural flexibility of the ranitidine molecule. Journal of Molecular Modeling, 2015, 21, 94.	0.8	1
38	Solvent effect on C60 tris-acid solubility: Light scattering, spectroscopic, electrochemical and computational studies. Diamond and Related Materials, 2021, 116, 108427.	1.8	1
39	Tris(1,10-phenanthroline-Î²2N,Nâ€²)ruthenium(II) bis(perchlorate). Acta Crystallographica Section E: Structure Reports Online, 2012, 68, m1570-m1571.	0.2	0