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	Adsorption of sulfur mustard on clean and water-saturated ZnO(10<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 757 Td (x calculations. Journal of Hazardous Materials, 2021, 402, 123503.	6.5	5
2	Solvent effect on C60 tris-acid solubility: Light scattering, spectroscopic, electrochemical and computational studies. Diamond and Related Materials, 2021, 116, 108427.	1.8	1
3	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
4	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
5	Single-walled carbon nanotubes in tetrahydrofuran solution: microsolvation from first-principles calculations. Journal of Molecular Modeling, 2019, 25, 206.	0.8	3
6	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
7	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
8	Intramolecular Hydrogen Bonds in Lowâ€Molecularâ€Weight Polyethylene Glycol. ChemPhysChem, 2016, 17, 1143-1153.	1.0	31
9	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
10	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
11	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
12	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
13	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
14	Triple helical collagen-like peptide interactions with selected polyphenolic compounds. RSC Advances, 2015, 5, 95443-95453.	1.7	14
15	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
16	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
17	Noncovalent functionalization of single-walled carbon nanotubes by aromatic diisocyanate molecules: A computational study. Chemical Physics Letters, 2014, 598, 10-16.	1.2	13
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	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
20	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
21	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
22	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
23	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
24	Cooperative effects in blue-shifted hydrogen bonded cluster of from first principles simulations. Chemical Physics, 2009, 361, 129-136.	0.9	10
25	Formic Acid Dimerization: Evidence for Species Diversity from First Principles Simulations. Journal of Physical Chemistry A, 2009, 113, 6266-6274.	1.1	23
26	Solvent effect on the blue shifted weakly H-bound F3 CHâ€¦FCD3 complex. Journal of Molecular Structure, 2008, 880, 64-68.	1.8	24
27	A Domino Annulation Reaction under Willgerodtâ^'Kindler Conditions. Journal of Organic Chemistry, 2008, 73, 4644-4649.	1.7	15
28	Formamide Dimers:â€‰ A Computational and Matrix Isolation Study. Journal of Physical Chemistry A, 2007, 111, 10552-10561.	1.1	59
29	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
30	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
31	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
32	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
33	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
34	Car-Parrinello Molecular Dynamics Study of a Blue-Shifted Intermolecular Weak-Hydrogen-Bond System. ChemPhysChem, 2005, 6, 1719-1724.	1.0	14
35	Ab Initio Studies of Electron Acceptor-Donor Interactions with Blue- and Red-Shifted Hydrogen Bonds. ChemPhysChem, 2005, 6, 1282-1292.	1.0	59
36	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

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37	CHâ‹¯B interactions in acetylene containing solutions: experimental and theoretical DFT studies. Journal of Molecular Structure, 2003, 645, 295-302.	1.8	6
38	Infrared studies of acetylene dissolved in liquefied Ar, Kr, N2, CO, and CO2. Journal of Molecular Structure, 2002, 614, 305-313.	1.8	18
39	Unusual spectroscopic properties of CF3H dissolved in liquified Ar, N2, CO, and CO2. Chemical Physics Letters, 2002, 352, 301-310.	1.2	69