Andrea Alparone

List of Publications by Year
in descending order

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68	1,166	361413	454955
papers	citations	20 h-index	30 g-index

70	70	70	1125
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Linear and nonlinear optical properties of nucleic acid bases. Chemical Physics, 2013, 410, 90-98.	1.9	72
2	Ab Initio Study of the Structure and Polarizability of Sulfur Clusters, Sn(n= 2â^'12). Journal of Physical Chemistry A, 2001, 105, 9489-9497.	2.5	59
3	Tautomerism and polarizability in uracil: coupled cluster and density-functional theory study. Chemical Physics, 2004, 303, 27-36.	1.9	48
4	Electronic and vibrational polarizabilities of the twenty naturally occurring amino acids. Biophysical Chemistry, 2008, 132, 139-147.	2.8	44
5	Response electric properties of Î±-helix polyglycines: A CAM-B3LYP DFT investigation. Chemical Physics Letters, 2013, 563, 88-92.	2.6	44
6	Theoretical study of the structure and torsional potential of pyrrole oligomers. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 25-32.	1.7	41
7	(Hyper)polarizability of chalcogenophenes C4H4X (X = O, S, Se, Te) Conventional ab initio and density functional theory study. Computational and Theoretical Chemistry, 1998, 431, 59-78.	1.5	39
8	Anharmonic vibrational spectroscopic investigation of malonaldehyde. Chemical Physics, 2003, 290, 15-25.	1.9	39
9	Theoretical Investigation of the (Hyper)polarizabilities of Pyrrole Homologues C4H4XH (X = N, P, As,) Tj ETQq1 1 0.784314 rgBT /Over 110, 5909-5918.	2.5	38
10	Comparative study of CCSD(T) and DFT methods: Electronic (hyper)polarizabilities of glycine. Chemical Physics Letters, 2011, 514, 21-25.	2.6	37
11	Electronic Polarizability as a Predictor of Biodegradation Rates of Dimethylnaphthalenes. AnAb Initioand Density Functional Theory Study. Environmental Science & Technology, 2007, 41, 1646-1652.	10.0	34
12	Validation of semiempirical PM6 method for the prediction of molecular properties of polycyclic aromatic hydrocarbons and fullerenes. Chemical Physics Letters, 2008, 460, 151-154.	2.6	33
13	Theoretical determination of the vibrational and electronic (hyper)polarizabilities of C4H4X (X=O, S,) Tj ETQq1 1 0.784314 rgBT /Over	2.8	32
14	Electronic properties of neuroleptics: ionization energies of benzodiazepines. Journal of Molecular Modeling, 2011, 17, 281-287.	1.8	27
15	Ab initio and density functional theory calculations of the dipole polarizabilities of ethene, benzene and naphthalene. Computational and Theoretical Chemistry, 1998, 422, 179-190.	1.5	26
16	Conformational properties of thiophene oligomers. Journal of Heterocyclic Chemistry, 2000, 37, 847-853.	2.6	26
17	Non-planarity and solvent effects on structural and polarizability properties of cytosine tautomers. Chemical Physics, 2005, 312, 261-274.	1.9	24
18	Second hyperpolarisability of furan homologues C4H4X (X=O, S, Se, Te): ab initio HF and DFT study. Chemical Physics Letters, 2000, 332, 175-180.	2.6	22

#	Article	IF	Citations
19	Electronic dipole polarizability and hyperpolarizability of formic acid. Chemical Physics Letters, 2005, 409, 288-294.	2.6	22
20	Computational study on dipole moment, polarizability and second hyperpolarizability of nitronaphthalenes. Computational and Theoretical Chemistry, 2008, 856, 105-111.	1.5	20
21	Prediction of mutagenic activity of nitronaphthalene isomers by infrared and Raman spectroscopy. Journal of Hazardous Materials, 2008, 154, 1158-1165.	12.4	20
22	Density functional theory Raman spectra of cyclic selenium clusters Sen (n=5â€“12). Computational and Theoretical Chemistry, 2012, 988, 81-85.	2.5	20
23	Dipole (hyper)polarizabilities of fluorinated benzenes: An ab initio investigation. Journal of Fluorine Chemistry, 2012, 144, 94-101.	1.7	20
24	Gas and solution phase electronic and vibrational (hyper)polarizabilities in the series formaldehyde, formamide and urea: CCSD(T) and DFT theoretical study. Chemical Physics Letters, 2005, 416, 282-288.	2.6	19
25	STRUCTURE, VIBRATIONAL PROPERTIES AND POLARIZABILITIES OF METHYLNAPHTHALENE ISOMERS. A QUANTUM-MECHANICAL APPROACH. Polycyclic Aromatic Compounds, 2007, 27, 65-94.	2.6	19
26	Ab initio study of the molecular structure, polarizability and first hyperpolarizability of 6-hydroxy-1-formylfulvene. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2873.	1.7	18
27	The role of electronic properties to the mutagenic activity of 1,6- and 3,6-dinitrobenzo[a]pyrene isomers. Journal of Hazardous Materials, 2009, 161, 1338-1346.	12.4	18
28	Theoretical investigation of the structure and conformational behaviour of small selenophene oligomers. Synthetic Metals, 1998, 95, 217-224.	3.9	17
29	Electronic properties of some nitrobenzo[a]pyrene isomers: a possible relationship to mutagenic activity. Journal of Molecular Modeling, 2008, 14, 489-497.	1.8	16
30	The PAH and Nitro-PAH Concentration Profiles in Size-Segregated Urban Particulate Matter and Soil in Traffic-Related Sites in Catania, Italy. Polycyclic Aromatic Compounds, 2012, 32, 439-456.	2.6	16
31	Structural, energetic and response electric properties of cyclic selenium clusters: an ab initio and density functional theory study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
32	Theoretical investigation of the dipole polarisability and second hyperpolarisability of cyclopentadiene homologues C4H4XH2 (X=C, Si, Ge, Sn). Chemical Physics, 2004, 298, 75-86.	1.9	13
33	Ab initio and DFT anharmonic spectroscopic investigation of 1,3-cyclopentadiene. Chemical Physics, 2006, 327, 127-136.	1.9	13
34	Theoretical study of the electronic (hyper)polarizabilities of amino acids in gaseous and aqueous phases. Computational and Theoretical Chemistry, 2011, 976, 188-190.	2.5	13
35	IR and Raman spectra of nitroanthracene isomers: Substitional effects based on density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 129-136.	3.9	12
36	Prediction of mutagenic activity of nitrophenanthrene and nitroanthracene isomers by simulated IR and Raman spectra. Chemosphere, 2013, 90, 158-163.	8.2	12

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37	Evolution of Electric Dipole (Hyper)polarizabilities of Î²-Strand Polyglycine Single Chains: An ab Initio and DFT Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 5184-5194.	2.5	12
38	The effect of secondary structures on the NLO properties of single chain oligopeptides: a comparison between Î²-strand and Î±-helix polyglycines. Physical Chemistry Chemical Physics, 2013, 15, 12958.	2.8	12
39	Second Harmonic Generation, Electrooptical Pockels Effect, and Static First-Order Hyperpolarizabilities of 2,2â€²-Bithiophene Conformers: An HF, MP2, and DFT Theoretical Investigation. Advances in Physical Chemistry, 2013, 2013, 1-8.	2.0	12
40	Static and Dynamic Electronic (Hyper)polarizabilities of Dimethylnaphthalene Isomers: Characterization of Spatial Contributions by Density Analysis. Scientific World Journal, The, 2013, 2013, 1-9.	2.1	12
41	Vibrational properties and first hyperpolarizability of cyclopentadiene homologues C4H4XH2 (X=C, Si,) Tj ETQq1 1 0.784314 rgBT /Over	1.5	11
42	Spectroscopic properties of neuroleptics: IR and Raman spectra of Risperidone (Risperdal) and of its mono- and di-protonated forms. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 631-639.	3.9	11
43	Raman DFT study of dimethylnaphthalenes: isomer identification and prediction of biodegradation rate coefficients. Structural Chemistry, 2012, 23, 1467-1474.	2.0	11
44	Electronic dipole polarizabilities of polychlorinated dibenzofurans and semiempirical PM6 level performance. Computational and Theoretical Chemistry, 2009, 894, 128.	1.5	10
45	Computational note on anharmonic infrared spectrum of naphthalene. Computational and Theoretical Chemistry, 2007, 847, 23-24.	1.5	8
46	Ionization energy and electron affinity of oligoglycines: a CAM-B3LYP density functional theory study. Monatshefte FÃ¼r Chemie, 2012, 143, 513-517.	1.8	8
47	Electron correlation effects and density analysis of the first-order hyperpolarizability of neutral guanine tautomers. Journal of Molecular Modeling, 2013, 19, 3095-3102.	1.8	8
48	Physicochemical characterization of environmental mutagens: 3-nitro-6-azabenzo[a]pyrene and its N-oxide derivative. Monatshefte FÃ¼r Chemie, 2012, 143, 1123-1132.	1.8	7
49	Nonlinear optical properties of fluorobenzenes: A Time-Dependent Hartreeâ€“Fock study. Computational and Theoretical Chemistry, 2013, 1013, 23-24.	2.5	7
50	Anharmonic IR and Raman spectra and electronic and vibrational (hyper)polarizabilities of barbituric, 2-thiobarbituric and 2-selenobarbituric acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 669-678.	3.9	5
51	Theoretical study on the static and dynamic first-order hyperpolarisabilities of adenine tautomers. Molecular Physics, 2014, 112, 1755-1760.	1.7	5
52	Structure and (Hyper)polarizabilities of Five-membered Heterocycles C4H4XH2 (X=C, Si, Ge, Sn). Journal of Chemical Research Synopses, 1999, , 238-239.	0.3	4
53	Structural, torsional, vibrational and response electric properties of 2,2â€²-bitellurophene rotamers. An ab initio and density functional theory investigation. Structural Chemistry, 2014, 25, 959-968.	2.0	4
54	Computational note on IR and Raman spectra of neutral and protonated forms of Aripiprazole (Abilify) and its metabolite Dehydroaripiprazole. Computational and Theoretical Chemistry, 2010, 955, 178-179.	1.5	3

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55	Nonlinear optical properties of benzofurobenzofurans. Journal of Heterocyclic Chemistry, 1997, 34, 195-201.	2.6	2
56	Computational note on the IR spectra of 7- and 9-hydroxyrisperidone isomers. Computational and Theoretical Chemistry, 2009, 911, 144.	1.5	2
57	Physicochemical characterization of neuroleptics. Relative stability of 7- and 9-hydroxyrisperidones and their protonated forms in gas phase and in solution. European Journal of Medicinal Chemistry, 2010, 45, 1367-1373.	5.5	2
58	Computational note on the structure and vibrational spectra of organic micropollutants: 1-Ethylnaphthalene and 2-ethylnaphthalene. Computational and Theoretical Chemistry, 2011, 965, 244-245.	2.5	2
59	Comment on: â€œFT-IR, FT-Raman and UV spectral investigation; computed frequency estimation analysis and electronic structure calculations on 1-nitronaphthaleneâ€•by M. Govindarajan and M. Karabacak [Spectrochim. Acta A 85 (2012) 251â€“260]. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 479-480.	3.9	2
60	Solvation Effects on the Static and Dynamic First-Order Electronic and Vibrational Hyperpolarizabilities of Uracil: A Polarized Continuum Model Investigation. Scientific World Journal, The, 2013, 2013, 1-7.	2.1	2
61	A Quantum Chemical Study on Structures and Electronic (Hyper)polarizabilities of 2,2â€²-Biselenophene Rotamers. , 2013, 2013, 1-5.		2
62	Vibrational and Electronic Spectra of Silole: A Theoretical PT2-DFT Anharmonic and TD-DFT Study. Journal of Applied Spectroscopy, 2014, 81, 320-327.	0.7	2
63	Second harmonic generation and electro-optical Pockels effect of 1- and 3-nitro-6-azabenzo[a]pyrene N-oxide isomers: A Hartreeâ€“Fock and Coulomb-attenuating density functional theory investigation. Journal of Chemical Sciences, 2014, 126, 701-710.	1.5	2
64	Computational analyses of virtual proteolytic fragments generated by naphthalene 1,2-dioxygenase. In search of native-like conformation and function. Molecular Simulation, 2007, 33, 231-237.	2.0	1
65	DFT calculation of geometrical structure and electronic absorption spectra for neutral, mono-, and diprotonated forms of Risperidone (Risperdal). Journal of Applied Spectroscopy, 2012, 79, 535-539.	0.7	1
66	Infrared and Raman Spectra of and Isotopomers: A DFT-PT2 Anharmonic Study. Journal of Chemistry, 2013, 2013, 1-8.	1.9	1
67	Anharmonic Spectroscopic Investigation of Tellurophene and Its Perdeuterated Isotopomer: Application of Second-Order Perturbation Theory. Journal of Quantum Chemistry, 2014, 2014, 1-8.	0.9	0
68	A systematic study of the linear and non-linear optical properties of small molecules and clusters. , 2006, , 294-307.		0