Aggelos Avramopoulos

List of Publications by Year
in descending order

60	1,209	304602	395590
papers	citations	22 h-index	33 g-index

63	63	63	1417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Linear and Nonlinear Optical Properties of [60]Fullerene Derivatives. Journal of Physical Chemistry A, 2009, 113, 1159-1170.	1.1	102
2	The Dipole Moment, Polarizabilities, and First Hyperpolarizabilities of HArF. A Computational and Comparative Study. Journal of the American Chemical Society, 2004, 126, 6179-6184.	6.6	100
3	Electronic and Vibrational Polarizabilities and Hyperpolarizabilities of Azoles: A Comparative Study of the Structureâ^'Polarization Relationship. Journal of Physical Chemistry A, 2003, 107, 4172-4183.	1.1	60
4	Tailoring Colors by O Annulation of Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2017, 23, 2363-2378.	1.7	55
5	Electronic and vibrational contributions to first hyperpolarizability of donorâ€“acceptor-substituted azobenzene. Journal of Chemical Physics, 2010, 133, 244308.	1.2	51
6	Linear and nonlinear optical properties of a series of Ni-dithiolene derivatives. Journal of Chemical Physics, 2009, 131, 134312.	1.2	50
7	Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. Journal of Computational Chemistry, 2013, 34, 1775-1784.	1.5	46
8	Strong interactions through the Xâ‹¯Auâ€“Y bridge: the Au bond?. Chemical Physics Letters, 2003, 370, 765-769.	1.2	42
9	Linear and nonlinear optical properties of triphenylamine-functionalized C60: insights from theory and experiment. Physical Chemistry Chemical Physics, 2010, 12, 373-381.	1.3	42
10	Advantages and limitations of classic and 3D QSAR approaches in nano-QSAR studies based on biological activity of fullerene derivatives. Journal of Nanoparticle Research, 2016, 18, 256.	0.8	37
11	Size-dependent electronic properties of nanomaterials: How this novel class of nanodescriptors supposed to be calculated?. Structural Chemistry, 2017, 28, 635-643.	1.0	36
12	Static electronic and vibrational first hyperpolarizability of meta-dinitrobenzene as studied by quantum chemical calculations. Computational and Theoretical Chemistry, 2009, 907, 46-50.	1.5	34
13	Vibrational corrections to electric properties of relativistic molecules: The coinage metal hydrides. Journal of Chemical Physics, 2001, 114, 198.	1.2	30
14	Calculation of the Microscopic and Macroscopic Linear and Nonlinear Optical Properties of Acetonitrile:â€‰ I. Accurate Molecular Properties in the Gas Phase and Susceptibilities of the Liquid in Onsager's Reaction-Field Model. Journal of Physical Chemistry A, 2003, 107, 3907-3917.	1.1	28
15	Electronic and vibrational linear and nonlinear polarizabilities of Li@C₆₀ and [Li@C₆₀]⁺. Journal of Computational Chemistry, 2011, 32, 908-914.	1.5	26
16	Structural and static electric response properties of highly symmetric lithiated silicon cages: Theoretical predictions. Journal of Computational Chemistry, 2012, 33, 1068-1079.	1.5	26
17	Theoretical Modelling of Photoswitching of Hyperpolarisabilities in Ruthenium Complexes. Chemistry - A European Journal, 2013, 19, 15955-15963.	1.7	25
18	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Î¹-Opioid Receptor Complexes. Journal of Chemical Information and Modeling, 2014, 54, 2294-2308.	2.5	25

#	Article	IF	Citations
19	A Series of Novel Derivatives with Giant Second Hyperpolarizabilities, Based on Radiaannulenes, Tetrathiafulvalene, Nickel Dithiolene, and Their Lithiated Analogues. Journal of Physical Chemistry C, 2016, 120, 9419-9435.	1.5	25
20	A Computational Strategy for the Design of Photochromic Derivatives Based on Diarylethene and Nickel Dithiolene with Large Contrast in Nonlinear Optical Properties. Journal of Physical Chemistry C, 2020, 124, 4221-4241.	1.5	23
21	A Comparative Study of the Dipole Polarizability of Some Zn Clusters. Journal of Physical Chemistry B, 2005, 109, 18822-18830.	1.2	22
22	A Comprehensive Computational Study of the Interaction between Human Serum Albumin and Fullerenes. Journal of Physical Chemistry B, 2015, 119, 14971-14985.	1.2	22
23	Synthesis and non-linear optical properties of some novel nickel derivatives. Chemical Physics, 2010, 372, 33-45.	0.9	21
24	On the Electronic Structure of Hâˆ'Ngâˆ'Ngâˆ'F (Ng = Ar, Kr, Xe) and the Nonlinear Optical Properties of HXe₂F. Journal of Chemical Theory and Computation, 2010, 6, 3365-3372.	2.3	20
25	A Computational Study of the Interaction and Polarization Effects of Complexes Involving Molecular Graphene and C₆₀ or a Nucleobases. Journal of Physical Chemistry A, 2016, 120, 284-298.	1.1	20
26	The (hyper)polarizabilities of AuXeF and XeAuF. Chemical Physics Letters, 2009, 472, 185-189.	1.2	17
27	Linear and nonlinear optical properties of some organoxenon derivatives. Journal of Chemical Physics, 2007, 127, 214102.	1.2	16
28	Electronic spectrum of the confined auride ion. Physical Chemistry Chemical Physics, 2003, 5, 1096-1102.	1.3	15
29	Calculation of the Microscopic and Macroscopic Linear and Nonlinear Optical Properties of Liquid Acetonitrile. II. Local Fields and Linear and Nonlinear Susceptibilities in Quadrupolar Approximation. Journal of Physical Chemistry B, 2007, 111, 2546-2553.	1.2	14
30	Ni Dithiolenes â€“ A Theoretical Study on Structureâ€“Property Relationships. European Journal of Inorganic Chemistry, 2013, 2013, 4839-4850.	1.0	14
31	Systematic Molecular Dynamics, MMâ€“PBSA, and Ab Initio Approaches to the Saquinavir Resistance Mechanism in HIV-1 PR Due to 11 Double and Multiple Mutations. Journal of Physical Chemistry B, 2014, 118, 9538-9552.	1.2	14
32	A computational study of photonic materials based on Ni bis(dithiolene) fused with benzene, possessing gigantic second hyperpolarizabilities. Journal of Materials Chemistry C, 2018, 6, 91-110.	2.7	14
33	Relativistic effects on interaction-induced electric properties of weakly interacting systems: The HFâ€¦AuH dimer. Journal of Chemical Physics, 2002, 117, 10026-10038.	1.2	13
34	Trends in the electronic and vibrational contributions to the dipole moment, polarizabilities, and first and second hyperpolarizabilities of the hydrides of Li, Na and K. Molecular Physics, 2002, 100, 821-834.	0.8	12
35	Significant nonlinearâ€optical switching capacity in atomic clusters built from silicon and lithium: A combined ab initio and density functional study. Journal of Computational Chemistry, 2014, 35, 829-838.	1.5	12
36	Polarizabilities and second hyperpolarizabilities of ZnmCdnclusters. Molecular Physics, 2006, 104, 2027-2036.	0.8	11

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37	Linear and nonlinear electric properties and their dependence on the conformation and intramolecular H-bonding: A model study. Chemical Physics, 2006, 328, 33-44.	0.9	11
38	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. Advances in Experimental Medicine and Biology, 2017, 947, 303-324.	0.8	8
39	Linearâ€"Scaling Calculations of Linear and Nonlinear Optical Properties of [60]fullerene Derivatives. , 2009, , .		7
40	A Twisted Bayâ€Substituted Quaterrylene Phosphorescing in the <scp>NIR</scp> Spectral Region. Helvetica Chimica Acta, 2017, 100, e1700192.	1.0	7
41	Theoretical investigations of the IR spectroscopy of Ni(C2S2H2)2. A case study of the P_VMWCI2 algorithm including anharmonic effects. Physical Chemistry Chemical Physics, 2010, 12, 13746.	1.3	6
42	On the Stability, Electronic Structure, and Nonlinear Optical Properties of HXeOXeF and FXeOXeF. Journal of Physical Chemistry A, 2011, 115, 10226-10236.	1.1	6
43	On the vibrational linear and nonlinear optical properties of compounds involving noble gas atoms: HXeOXeH, HXeOXeF, and FXeOXeF. Journal of Computational Chemistry, 2013, 34, 1446-1455.	1.5	6
44	Computational investigation of fullerene-DNA interactions: Implications of fullereneâ€™s size and functionalization on DNA structure and binding energetics. Journal of Molecular Graphics and Modelling, 2017, 74, 177-192.	1.3	6
45	Computer Simulation of the Nonlinear Optical Properties of Langmuirâ€“Blodgett Films of a Squaraine Derivative. Journal of Physical Chemistry C, 2012, 116, 15449-15457.	1.5	5
46	In silico study of levodopa in hydrated lipid bilayers at the atomistic level. Journal of Molecular Graphics and Modelling, 2021, 107, 107972.	1.3	4
47	On the origin of the large electron correlation contribution to the hyperpolarizabilities of some diacetylene rare gas compounds. Journal of Chemical Physics, 2008, 129, 144308.	1.2	3
48	Critical assessment of density functional theory for computing vibrational (hyper)polarizabilities. , 2012, , .		3
49	Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays. Journal of Molecular Graphics and Modelling, 2015, 62, 138-149.	1.3	3
50	Stability and binding effects of silver(I) complexes at lipoxygenase-1. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 539-549.	2.5	3
51	Static second-hyperpolarizability of diffuse electron cyclic compounds M2A2 (Mâ€¯=â€¯Be, Mg, Ca; Aâ€¯=â€¯Li, Na,) Tj ETQq1 1 0.784	1.2	3
52	The Linear and Non-Linear Optical Properties of Some Noble Gas Compounds. AIP Conference Proceedings, 2007, , .	0.3	2
53	The effect of the vibrational contributions to the non-linear optical properties of small and medium size molecules. AIP Conference Proceedings, 2012, , .	0.3	2
54	Nonlinear optical response of some Boron-dipyrromethene dyes: An experimental and theoretical investigation. Materials Chemistry and Physics, 2022, 283, 126057.	2.0	2

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55	The effect of the vibrational contributions to the non-linear optical properties of small and medium size molecules. , 2012, , .		1
56	Far-Red to Near Infrared Emissive Aqueous Nanoparticles Based on a New Organic Material with Three BODIPY Dyes at the Periphery of the Core: A Combined Experimental and Theoretical Study. Electronic Materials, 2021, 2, 24-38.	0.9	1
57	Electronic contributions to linear and nonlinear electric properties in fullerene-based molecular systems. , 2012, , .		0
58	Chapter 8. Theoretical Studies of Interactions in Nanomaterials and Biological Systems. RSC Nanoscience and Nanotechnology, 2012, , 148-186.	0.2	0
59	Mechanisms of Polarization. Modeling and Optimization in Science and Technologies, 2014, , 83-92.	0.7	0
60	A theoretical study of the non-linear optical properties of a series of Ni-dithiolene derivatives. , 2015, , .		0