Panaghiotis E Karamanis

List of Publications by Year
in descending order

65	1,520	279701	330025
papers	citations	23 h-index	37 g-index

66	66	66	1064
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	How do the available density functionals perform on the calculation of eigenvalues of frontier to deeper orbitals? A metric space evaluation of experimental and quantum chemical findings. Chemical Physics, 2022, 561, 111600.	0.9	1
2	Electronic and magnetic properties of yttria-stabilized zirconia (6.7Âmol% in Y2O3) doped with Er3+ ions from first-principle computations. Journal of Materials Science, 2021, 56, 8014-8023.	1.7	0
3	Third order non-linear optical susceptibilities <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si24.svg"><mml:mrow><mml:msup><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mi>Ì‡</mml:mi></mml:mrow><mml:mfenced open="(") Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	1.2	1
4	Degradation of polar and non-polar pharmaceutical pollutants in water by solar assisted photocatalysis using hydrothermal TiO2-SnS2. Chemical Engineering Journal, 2020, 382, 122826.	6.6	37
5	From Pyridine Adduct of Borabenzene to (In)finite Graphene Architectures Functionalized with N â† B Dative Bonds. Prototype Systems of Strong One- and Two-Photon Quantum Transitions Triggering Large Nonlinear Optical Responses. Journal of Physical Chemistry C, 2020, 124, 21063-21074.	1.5	9
6	Polyaromatic Systems Combining Increasing Optical Gaps and Amplified Nonlinear Optical Properties. A Comprehensive Theoretical Study on B₃N₃ Doped Nanographenes. Journal of Physical Chemistry C, 2019, 123, 21135-21149.	1.5	11
7	Ab-initio calculations of the IR spectra of dicyanodiacetylene (C6N2) beyond the harmonic approximation. Chemical Physics Letters, 2019, 723, 155-159.	1.2	8
8	A new method to analyze and understand molecular linear and nonlinear optical responses via field-induced functions: a straightforward alternative to sum-over-states (SOS) analysis. Physical Chemistry Chemical Physics, 2019, 21, 6274-6286.	1.3	13
9	Theoretical Investigation of the Infrared Spectrum of 5â€Bromoâ€2,4â€pentadiynenitrile from a CCSD(T)/B3LYP Anharmonic Potential. ChemPhysChem, 2018, 19, 822-826.	1.0	4
10	Hirshfeld-based atomic population analysis of the B, N doping effect in zigzag graphene nanoribbons: $$pi$$Ï€ electron density as requirement to follow the B, N doping guidelines. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	4
11	Ab initio calculation of nonlinear optical properties for chiral carbon nanotubes. Second harmonic generation and dc-Pockels effect. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	4
12	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
13	Structures and Electric Properties of Semiconductor clusters. , 2017, , 1097-1137.		1
14	Quadratic nonlinear optical (NLO) properties of borazino (B₃N₃)-doped nanographenes. Journal of Materials Chemistry C, 2017, 5, 8273-8287.	2.7	33
15	Prediction of biodegradability of aromatics in water using QSAR modeling. Ecotoxicology and Environmental Safety, 2017, 139, 139-149.	2.9	20
16	Exploring the Linear Optical Properties of Borazine (B₃N₃) Doped Graphenes. 0D Flakes vs 2D Sheets. Journal of Physical Chemistry C, 2017, 121, 709-722.	1.5	24
17	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
18	Establishing the pivotal role of local aromaticity in the electronic properties of boron-nitride graphene lateral hybrids. Physical Chemistry Chemical Physics, 2016, 18, 25315-25328.	1.3	19

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19	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
20	Hirshfeldâ€based intrinsic polarizability density representations as a tool to analyze molecular polarizability. Journal of Computational Chemistry, 2015, 36, 1831-1843.	1.5	22
21	Electric Property Variations in Nanosized Hexagonal Boron Nitride/Graphene Hybrids. Journal of Physical Chemistry C, 2015, 119, 11872-11885.	1.5	28
22	Structures and Electric Properties of Semiconductor clusters. , 2015, , 1-41.		0
23	Unleashing the Quadratic Nonlinear Optical Responses of Graphene by Confining White-Graphene (h-BN) Sections in Its Framework. Journal of the American Chemical Society, 2014, 136, 7464-7473.	6.6	71
24	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
25	Comment on â€œPlanar tetra-coordinate carbon resulting in enhanced third-order nonlinear optical response of metal-terminated graphene nanoribbonsâ€• by G.-L. Chai, C.-S. Lin and W.-D. Cheng, J. Mater. Chem., 2012, 22, 11303. Journal of Materials Chemistry C, 2013, 1, 3035.	2.7	10
26	Electric response properties of neutral and charged Al13X (X=Li, Na, K) magic clusters. A comprehensive ab initio and density functional comparative study. Computational and Theoretical Chemistry, 2013, 1021, 114-123.	1.1	22
27	Second-Hyperpolarizability (Î³) Enhancement in Metal-Decorated Zigzag Graphene Flakes and Ribbons: The Size Effect. Journal of Physical Chemistry C, 2013, 117, 3134-3140.	1.5	32
28	Ab Initio Periodic Simulation of the Spectroscopic and Optical Properties of Novel Porous Graphene Phases. Journal of Physical Chemistry C, 2013, 117, 2222-2229.	1.5	33
29	Comment on â€œHow the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Grapheneâ€. Journal of Physical Chemistry C, 2013, 117, 721-724.	1.5	4
30	Is there any connection between the (Hyper) polarizabilities of the ground state structures of clusters and those of their low lying isomers? A case study of aluminum doped silicon clusters. , 2012, , .		0
31	The Importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: A critical analysis on prolate aluminum phosphide clusters. International Journal of Quantum Chemistry, 2012, 112, 2115-2125.	1.0	17
32	Fullereneâ€“C₆₀ in Contact with Alkali Metal Clusters: Prototype Nano-Objects of Enhanced First Hyperpolarizabilities. Journal of Physical Chemistry C, 2012, 116, 11808-11819.	1.5	66
33	Structures and Electric Properties of Semiconductor clusters. , 2012, , 723-759.		0
34	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
35	Evolution of Properties in Prolate (GaAs)nClusters. Journal of Physical Chemistry C, 2011, 115, 97-107.	1.5	30
36	Doping-enhanced hyperpolarizabilities of silicon clusters: A global ab initio and density functional theory study of Si10 (Li, Na, K)n (n = 1, 2) clusters. Journal of Chemical Physics, 2011, 135, 044511.	1.2	69

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37	An ab initio study of CX₃â€substitution (Xâ€‰=â€‰H, F, Cl, Br, I) effects on the static electric polarizability and hyperpolarizability of diacetylene. Journal of Physical Organic Chemistry, 2011, 24, 588-599.	0.9	41
38	On the shape dependence of cluster (hyper)polarizabilities. A combined ab initio and DFT study on large fullereneâ€“like gallium arsenide semiconductor clusters. International Journal of Quantum Chemistry, 2011, 111, 788-796.	1.0	14
39	A critical analysis of the performance of new generation functionals on the calculation of the (hyper) polarizabilities of clusters of varying stoichiometry: Test case the SimGen (m+n=7, n=0â€“7) clusters. Chemical Physics Letters, 2010, 498, 134-139.	1.2	19
40	Doping effects on the electric response properties of silicon clusters: A global structureâ€“property investigation of AlSiâ^'1 clusters (n= 3â€“10). Chemical Physics Letters, 2010, 500, 59-64.	1.2	17
41	Polarizabilities and Hyperpolarizabilities of Binary Semiconductor Clusters. , 2009, , .		0
42	How large are the microscopic electronic dipole (hyper)polarizabilities of CdnTen bare clusters compared to those of CdnSn and CdnSen? A systematic ab initio study. Chemical Physics Letters, 2009, 474, 162-167.	1.2	18
43	Computational Quantum Chemistry: From Atoms and Molecules to Clusters and Nano-objects. , 2009, , .		0
44	Surface enhanced Raman spectroscopy (SERS) and density functional theory (DFT) study for understanding the regioselective adsorption of pyrrolidinone on the surface of silver and gold colloids. Journal of Molecular Structure, 2009, 935, 32-38.	1.8	62
45	Structures and composition-dependent polarizabilities of open- and closed-shell<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub> clusters. Physical Review A, 2009, 80, .	1.0	20
46	The polarizabilities of small stoichiometric aluminum phosphide clusters AlnPn (n=2â€“9). Ab initio and density functional investigation. Chemical Physics Letters, 2008, 457, 137-142.	1.2	22
47	Structure, stability, dipole polarizability and differential polarizability in small gallium arsenide clusters from all-electronab initioand density-functional-theory calculations. Physical Review A, 2008, 77, .	1.0	124
48	Electric Dipole (Hyper)polarizabilities of Selected X₂Y₂ and X₃Y₃ (X = Al, Ga, In and Y = P, As): IIIâ^'V Semiconductor Clusters. An ab Initio Comparative Study. Journal of Physical Chemistry A, 2008, 112, 13662-13671.	1.1	23
49	Polarizability evolution on natural and artificial low dimensional binary semiconductor systems: A case study of stoichiometric aluminum phosphide semiconductor clusters. Journal of Chemical Physics, 2008, 129, 094708.	1.2	20
50	Correlations between bonding, size, and second hyperpolarizability (Î³) of small semiconductor clusters: Ab initio study on AlnPn clusters with n=2, 3, 4, 6, and 9. Journal of Chemical Physics, 2008, 128, 154323.	1.2	33
51	Hyperpolarizability of GaAs dimer is not negative. Journal of Chemical Physics, 2007, 126, 154316.	1.2	74
52	Electric Dipole Polarizability of Aluminum Phosphide Clusters Al[sub n]P[sub n] (nâ€‰=â€‰2â€“9) and Electron Delocalization. AIP Conference Proceedings, 2007, , .	0.3	0
53	Ab initio finite field (hyper)polarizability computations on stoichiometric gallium arsenide clusters GanAsnâ€^(n=2â€“9). Journal of Chemical Physics, 2007, 127, 094706.	1.2	38
54	A critical analysis of the performance of conventional ab initio and DFT methods in the computation of Si6 ground state. Chemical Physics, 2007, 331, 417-426.	0.9	20

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55	Molecular geometry and polarizability of small cadmium selenide clusters from all-electronab initioand Density Functional Theory calculations. Journal of Chemical Physics, 2006, 124, 071101.	1.2	74
56	Basis set and electron correlation effects in all-electron ab initio calculations of the static dipole polarizability of small cadmium selenide clusters, (CdSe)n, n=1,2,3,4. Chemical Physics, 2006, 331, 19-25.	0.9	33
57	How Important are High-Level ab initio Treatments for the Interaction Dipole Moment and Polarizability of Hene?. Computing Letters, 2005, 1, 117-121.	0.5	9
58	Effect of the relative orientation of the CN moieties on the static electric (hyper)polarizability of (CN)2. Molecular Physics, 2004, 102, 13-21.	0.8	4
59	Single (Câ€“C) and triple (C˜†C) bond-length dependence of the static electric polarizability and hyperpolarizability of Hâ€“Cˆ†Câ€“Cˆ†Câ€“H. Chemical Physics Letters, 2003, 376, 403-410.	1.2	63
60	Static electric dipole polarizability and hyperpolarizability of fluorodiacetyleneâˆ†. Computational and Theoretical Chemistry, 2003, 621, 157-162.	1.5	20
61	Electric quadrupole and hexadecapole moments for X2C?CX2, X = H, F, Cl, Br, and I. International Journal of Quantum Chemistry, 2002, 90, 483-490.	1.0	8
62	Finite-field MÃ¸llerâ€“Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As2. Chemical Physics, 2001, 269, 137-146.	0.9	14
63	Electric dipole and quadrupole moment and dipole polarizability of CS, SiO and SiS. Molecular Physics, 2000, 98, 481-491.	0.8	29
64	Electric dipole and quadrupole moment and dipole polarizability of CS, SiO and SiS. Molecular Physics, 2000, 98, 481-491.	0.8	5
65	Electric Dipole Polarizability of As4, a Challenging Problem for Both Experiment and Theory. Journal of Physical Chemistry A, 1998, 102, 1237-1240.	1.1	26