

Demetrios Xenides

List of Publications by Year in descending order

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34
papers

873
citations

567281

15
h-index

501196

28
g-index

35
all docs

35
docs citations

35
times ranked

557
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. <i>Chemical Physics</i> , 2022, 561, 111600.	1.9	1
2	How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. <i>Journal of Physics: Conference Series</i> , 2021, 1730, 012126.	0.4	0
3	From Pyridine Adduct of Borabenzene to (In)finite Graphene Architectures Functionalized with N $\hat{\alpha}$ ' B Dative Bonds. Prototype Systems of Strong One- and Two-Photon Quantum Transitions Triggering Large Nonlinear Optical Responses. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21063-21074.	3.1	9
4	Comparison of high-level post-Hartree-Fock and DFT methods on the calculation of interaction-induced electric properties of Kr $\hat{\alpha}$ He. <i>Chemical Physics</i> , 2011, 382, 80-87.	1.9	21
5	Trends of the bonding effect on the performance of DFT methods in electric properties calculations: A pattern recognition and metric space approach on some XY ₂ (X = O, S and Y = H, O, F, S,) <i>Tj ETQq1 1.0.7843 14 rgBT / Qv</i>	1.0	14
6	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=0 $\hat{\alpha}$ 7) clusters. <i>Chemical Physics Letters</i> , 2010, 498, 134-139.	2.6	19
7	Finding the Pattern in the Space of ab initio and DFT Theoretical Descriptions: A Pattern Recognition and Metric Space Approach Based on the Electric Response Properties of the Open and Ring Isomers of XO ₂ (X $\hat{\alpha}$ O, S), 2009, ,		0
8	Computational Quantum Chemistry: From Atoms and Molecules to Clusters and Nano-objects. , 2009, ,		0
9	The polarizabilities of small stoichiometric aluminum phosphide clusters Al _n P _n (n=2 $\hat{\alpha}$ 9). Ab initio and density functional investigation. <i>Chemical Physics Letters</i> , 2008, 457, 137-142.	2.6	22
10	Polarizability evolution on natural and artificial low dimensional binary semiconductor systems: A case study of stoichiometric aluminum phosphide semiconductor clusters. <i>Journal of Chemical Physics</i> , 2008, 129, 094708.	3.0	20
11	Synchronization in complex systems following a decision based queuing process: rhythmic applause as a test case. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2008, 2008, P07017.	2.3	8
12	Static electric polarizability and hyperpolarizability of sodium clusters: The case of the sodium tetramer. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2008, 7, 431-442.	0.2	2
13	Electric polarizabilities of the C _x Si _{4-x} (0 $\hat{\alpha}$ 1/2 x $\hat{\alpha}$ 1/2 4) clusters. A conventional and time-dependent density functional theory study. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2008, 7, 287-296.	0.2	0
14	Electric Dipole Polarizability of Aluminum Phosphide Clusters Al _n P _n (n $\hat{\alpha}$ 2 $\hat{\alpha}$ 9) and Electron Delocalization. <i>AIP Conference Proceedings</i> , 2007, ,	0.4	0
15	Ab Initio QM $\hat{\alpha}$ MM Simulations of Water and Hydrated Cations. <i>AIP Conference Proceedings</i> , 2007, ,	0.4	0
16	On the performance of DFT methods in (hyper)polarizability calculations: N ₄ (Td) as a test case. <i>Computational and Theoretical Chemistry</i> , 2007, 804, 41-46.	1.5	15
17	Molecular geometry, charge distribution and polarization in platinum nitrides. An ab initio and density functional theory study of PtNN, PtPtNN, NPtPtN, and NNPtNN. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2006, 6, 201-209.	0.2	2
18	Hydrogen bonding in liquid water: An ab initio QM/MM MD simulation study. <i>Journal of Molecular Liquids</i> , 2006, 123, 61-67.	4.9	63

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19	(Hyper)polarizability dependence on the interatomic distance of N ₄ (Td): Fourth order polynomials and third order derivatives. Computational and Theoretical Chemistry, 2006, 764, 41-46.	1.5	8
20	Ab initio quantum mechanical charge field (QMCF) molecular dynamics: a QM/MM $\hat{=}$ MD procedure for accurate simulations of ions and complexes. Theoretical Chemistry Accounts, 2006, 115, 77-85.	1.4	183
21	Electric polarizability and hyperpolarizability of BrCl(X ¹ $\hat{=}$ +). Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 3629-3638.	1.5	11
22	Interaction dipole moment, polarizability and hyperpolarizability in the KrXe heterodiatom. Chemical Physics, 2005, 309, 271-275.	1.9	37
23	On the performance of DFT methods on electric polarizability and hyperpolarizability calculations for the lithium tetramer. Computing Letters, 2005, 1, 246-252.	0.5	15
24	Structure and ultrafast dynamics of liquid water: A quantum mechanics/molecular mechanics molecular dynamics simulations study. Journal of Chemical Physics, 2005, 122, 174506.	3.0	106
25	New basis sets for xenon and the interaction polarizability of two xenon atoms. Chemical Physics Letters, 2004, 396, 59-65.	2.6	43
26	Electric Quadrupole and Hexadecapole Moment, Dipole and Quadrupole Polarizability, Second Electric Dipole Hyperpolarizability for P ₂ , and a Comparative Study of Molecular Polarization in N ₂ , P ₂ , and As ₂ . Journal of Physical Chemistry A, 2003, 107, 712-719.	2.5	23
27	Electric Multipole Moments and (Hyper)Polarizability of X ¹ $\hat{=}$ X, X = F, Cl, Br and I. International Journal of Molecular Sciences, 2003, 4, 263-271.	4.1	7
28	How does protonation affect the electron density of ozone?. Molecular Physics, 2002, 100, 1057-1059.	1.7	1
29	Dipole, dipole $\hat{=}$ quadrupole, and dipole $\hat{=}$ octopole polarizability of adamantane, C ₁₀ H ₁₆ , from refractive index measurements, depolarized collision-induced light scattering, conventionalab initioand density functional theory calculations. Journal of Chemical Physics, 2001, 115, 7957-7967.	3.0	92
30	How does the closing of the ring affect the electric properties of sulphur dioxide? A comparison with the open and closed form of ozone. Journal of Chemical Physics, 2001, 115, 7953-7956.	3.0	10
31	Basis set and electron correlation effects on the first and second static hyperpolarizability of SO ₂ . Chemical Physics Letters, 2000, 319, 618-624.	2.6	55
32	Electric dipole and quadrupole moment and dipole polarizability of CS, SiO and SiS. Molecular Physics, 2000, 98, 481-491.	1.7	29
33	Enhanced Linear and Nonlinear Polarizabilities for the Li ₄ Cluster. How Satisfactory Is the Agreement between Theory and Experiment for the Static Dipole Polarizability?. Journal of Physical Chemistry A, 1999, 103, 4590-4593.	2.5	49
34	On the dipole polarizability of the cyclic form of ozone. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, L951-L954.	1.5	7