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	Ab initio quantum mechanical charge field (QMCF) molecular dynamics: a QM/MM â€“ MD procedure for accurate simulations of ions and complexes. Theoretical Chemistry Accounts, 2006, 115, 77-85.	1.4	183
2	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
3	Dipole, dipoleâ€“quadrupole, and dipoleâ€“octopole polarizability of adamantane, C10H16, 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
4	Hydrogen bonding in liquid water: An ab initio QM/MM MD simulation study. Journal of Molecular Liquids, 2006, 123, 61-67.	4.9	63
5	Basis set and electron correlation effects on the first and second static hyperpolarizability of SO2. Chemical Physics Letters, 2000, 319, 618-624.	2.6	55
6	Enhanced Linear and Nonlinear Polarizabilities for the Li4Cluster. 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
7	New basis sets for xenon and the interaction polarizability of two xenon atoms. Chemical Physics Letters, 2004, 396, 59-65.	2.6	43
8	Interaction dipole moment, polarizability and hyperpolarizability in the KrXe heterodiatom. Chemical Physics, 2005, 309, 271-275.	1.9	37
9	Electric dipole and quadrupole moment and dipole polarizability of CS, SiO and SiS. Molecular Physics, 2000, 98, 481-491.	1.7	29
10	Electric Quadrupole and Hexadecapole Moment, Dipole and Quadrupole Polarizability, Second Electric Dipole Hyperpolarizability for P2, and a Comparative Study of Molecular Polarization in N2, P2, and As2. Journal of Physical Chemistry A, 2003, 107, 712-719.	2.5	23
11	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.	2.6	22
12	Comparison of high-level post-Hartreeâ€“Fock and DFT methods on the calculation of interaction-induced electric properties of Krâ€“He. Chemical Physics, 2011, 382, 80-87.	1.9	21
13	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.	3.0	20
14	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.	2.6	19
15	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
16	On the performance of DFT methods in (hyper)polarizability calculations: N4 (Td) as a test case. Computational and Theoretical Chemistry, 2007, 804, 41-46.	1.5	15
17	Trends of the bonding effect on the performance of DFT methods in electric properties calculations: A pattern recognition and metric space approach on some XY₂ (X = O, S and Y = H, O, F, S,) Tj ETQq1 1 0.784314 rgBT /Ov	1.8	14
18	Electric polarizability and hyperpolarizability of BrCl(X1Î£+). Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 3629-3638.	1.5	11

#	Article	IF	Citations
19	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
20	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.	3.1	9
21	(Hyper)polarizability dependence on the interatomic distance of N4 (Td): Fourth order polynomials and third order derivatives. Computational and Theoretical Chemistry, 2006, 764, 41-46.	1.5	8
22	Synchronization in complex systems following a decision based queuing process: rhythmic applause as a test case. Journal of Statistical Mechanics: Theory and Experiment, 2008, 2008, P07017.	2.3	8
23	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
24	Electric Multipole Moments and (Hyper)Polarizability of Xâ€"Câ‰¡Câ€"X, X = F, Cl, Br and I. International Journal of Molecular Sciences, 2003, 4, 263-271.	4.1	7
25	Molecular geometry, charge distribution and polarization in platinum nitrides. An ab initio and density functional theory study of PtNN, PtPtNN, NPtPtN, and NNPtNN. Journal of Computational Methods in Sciences and Engineering, 2006, 6, 201-209.	0.2	2
26	Static electric polarizability and hyperpolarizability of sodium clusters: The case of the sodium tetramer. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 431-442.	0.2	2
27	How does protonation affect the electron density of ozone?. Molecular Physics, 2002, 100, 1057-1059.	1.7	1
28	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.	1.9	1
29	Electric Dipole Polarizability of Aluminum Phosphide Clusters Al[sub n]P[sub n] (nâ€‰=â€‰2â€"9) and Electron Delocalization. AIP Conference Proceedings, 2007, , .	0.4	0
30	Ab Initio QMâ•MM Simulations of Water and Hydrated Cations. AIP Conference Proceedings, 2007, , .	0.4	0
31	Electric polarizabilities of the CxSi4-x (0 â©½ x â©½ 4) clusters. A conventional and time-dependent density functional theory study. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 287-296.	0.2	0
32	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[sub 2] (Xâ€‰=â€‰O,S). , 2009, , .		0
33	Computational Quantum Chemistry: From Atoms and Molecules to Clusters and Nano-objects. , 2009, , .		0
34	How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. Journal of Physics: Conference Series, 2021, 1730, 012126.	0.4	0