

Kiet A Nguyen

List of Publications by Year in descending order

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52
papers

21,156
citations

212478

28
h-index

198040

52
g-index

52
all docs

52
docs citations

52
times ranked

17301
citing authors

#	ARTICLE	IF	CITATIONS
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	1.5	19,020
2	Ground state electronic structures and spectra of zinc complexes of porphyrin, tetraazaporphyrin, tetrabenzoporphyrin, and phthalocyanine: A density functional theory study. Journal of Chemical Physics, 2001, 114, 10757-10767.	1.2	212
3	Observation and Interpretation of Annulated Porphyrins: A Study on the Photophysical Properties of meso-Tetraphenylmetalporphyrins. Journal of Physical Chemistry A, 2003, 107, 11331-11339.	1.1	160
4	A dual-level Shepard interpolation method for generating potential energy surfaces for dynamics calculations. Journal of Chemical Physics, 1995, 103, 5522-5530.	1.2	142
5	Understanding Structural and Optical Properties of Nanoscale CdSe Magic-Size Quantum Dots: Insight from Computational Prediction. Journal of Physical Chemistry C, 2010, 114, 16197-16209.	1.5	115
6	TDDFT Study of One- and Two-Photon Absorption Properties of Donor-Acceptor Chromophores. Journal of Physical Chemistry B, 2005, 109, 1803-1814.	1.2	101
7	Analysis of Absorption Spectra of Zinc Porphyrin, Zinc meso-Tetraphenylporphyrin, and Halogenated Derivatives. Journal of Physical Chemistry A, 2002, 106, 10285-10293.	1.1	81
8	Reaction-path dynamics in curvilinear internal coordinates including torsions. Journal of Chemical Physics, 1996, 104, 6491-6496.	1.2	74
9	Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins. Journal of Chemical Physics, 1999, 110, 9135-9144.	1.2	68
10	A density functional theory study of phosphorescence and triplet-triplet absorption for nonlinear absorption chromophores. Journal of Chemical Physics, 2002, 117, 7128-7136.	1.2	67
11	Calculation of two-photon absorption spectra of donor-acceptor compounds in solution using quadratic response time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 094103.	1.2	63
12	The Inversion of Bicyclobutane and Bicyclodiazoxane. Journal of the American Chemical Society, 1994, 116, 9241-9249.	6.6	58
13	Isomerization Of Bicyclo[1.1.0]butane to Butadiene. Journal of the American Chemical Society, 1995, 117, 3835-3847.	6.6	55
14	Effect of hydration and dimerization of the formamidine rearrangement. Journal of the American Chemical Society, 1991, 113, 1596-1600.	6.6	51
15	Triplet Excited States of Free-Base Porphin and Its β^2 -Octahalogenated Derivatives. Journal of Physical Chemistry A, 2000, 104, 4748-4754.	1.1	51
16	Computational Prediction of Structures and Optical Excitations for Nanoscale Ultrasmall ZnS and CdSe Clusters. Journal of Chemical Theory and Computation, 2013, 9, 3581-3596.	2.3	51
17	Stabilization of β^+ positive charge by silicon, germanium, or tin. Organometallics, 1991, 10, 2798-2803.	1.1	50
18	Jahn-Teller triplet excited state structures and spectra of zinc complexes of porphyrin and phthalocyanine: A density functional theory study. Journal of Chemical Physics, 2003, 118, 5802-5810.	1.2	50

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19	The structure and bonding in group IV [1.1.1]Propellanes. <i>Polyhedron</i> , 1991, 10, 1247-1264.	1.0	48
20	Calculation of One- and Two-Photon Absorption Spectra of Thiolated Gold Nanoclusters using Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2809-2821.	2.3	47
21	The performance and relationship among range-separated schemes for density functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 074109.	1.2	43
22	Effects of Conjugation in Length and Dimension on Spectroscopic Properties of Fluorene-Based Chromophores from Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13172-13182.	1.1	42
23	Structures and bonding of Group IVA sulfur and oxygen propellane derivatives. <i>Journal of the American Chemical Society</i> , 1991, 113, 7924-7929.	6.6	40
24	Ground and Triplet Excited Structures and Spectroscopic Properties of Halogenated Zincmeso-Tetraphenylporphyrin. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9378-9382.	1.1	37
25	Analysis of nonlinear optical properties in donor-acceptor materials. <i>Journal of Chemical Physics</i> , 2014, 140, 184308.	1.2	32
26	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 507-518.	1.1	31
27	Structure, Bonding, and Stability of Small Boron-Lithium Clusters. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1608-1614.	1.1	29
28	One- and Two-Photon Spectra of Platinum Acetylide Chromophores: A TDDFT Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13943-13952.	1.1	28
29	Addition of a Phenyl Phosphinidene Complex to Conjugated Dienes. <i>Organometallics</i> , 1999, 18, 796-799.	1.1	27
30	Calculation of One-Photon and Two-Photon Absorption Spectra of Porphyrins Using Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1094-1106.	2.3	27
31	Theoretical studies of spin-forbidden radiationless decay in polyatomic systems. II. Radiationless decay of N_2O_2 . <i>Journal of Chemical Physics</i> , 1993, 98, 3845-3849.	1.2	26
32	Analytical energy gradients of Coulomb-attenuated time-dependent density functional methods for excited states. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2247-2255.	1.0	22
33	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of N_2O_2 . <i>Journal of Physical Chemistry A</i> , 1997, 101, 4283-4289.	1.1	21
34	Effects of conjugation in length and dimension on two-photon properties of fluorene-based chromophores. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 167-175.	0.5	19
35	Systematic survey of cyclic silicon-oxygen compounds. <i>Journal of the American Chemical Society</i> , 1991, 113, 5998-6001.	6.6	18
36	Photoinduced Hydrogen Atom Transfer of Free-Base Porphin. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4549-4552.	1.1	18

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37	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. <i>Journal of Chemical Physics</i> , 2015, 142, 234305.	1.2	18
38	Stability of Hyperlithiated Borides. <i>Journal of Physical Chemistry A</i> , 1999, 103, 710-715.	1.1	15
39	Ab Initio Study of the Thermal Isomerization of Tricyclo[3.1.0.0 ^{2,6}]hexane to (Z,Z)-1,3-Cyclohexadiene through the (E,Z)-1,3-Cyclohexadiene Intermediate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 198-203.	1.1	14
40	Alternative Mechanisms in Hydrogen Production by Aluminum Anion Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 152-161.	2.3	13
41	Systematic Study of Structure, Stability, and Electronic Absorption of Tetrahedral CdSe Clusters with Carboxylate and Amine Ligands. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6704-6712.	1.1	10
42	Theoretical Prediction of Optical Absorption and Emission in Thiolated Gold Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6472-6481.	1.1	9
43	Systematic Study of the Properties of CdS Clusters with Carboxylate Ligands Using a Deep Neural Network Potential Developed with Data from Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10472-10481.	1.1	9
44	Matrix-infrared spectra of structural isomers of the phosphorus oxysulfide P4S3O. <i>Inorganic Chemistry</i> , 1990, 29, 5096-5100.	1.9	7
45	A Theoretical Investigation of the Structure and Optical Properties of a Silver Cluster in Solid Form and in Solution. <i>Journal of Physical Chemistry A</i> , 2017, 121, 326-333.	1.1	7
46	Computational design of two-photon active organic molecules for infrared responsive materials. <i>Journal of Materials Chemistry C</i> , 2020, 8, 9867-9873.	2.7	7
47	Isomers on the Si ₂ CH ₄ ⁺ Potential Energy Surface. <i>Organometallics</i> , 1996, 15, 5391-5398.	1.1	5
48	Calculations of One- and Two-Photon Absorption Spectra for Molecular Metal Chalcogenide Clusters with Electron-Acceptor Ligands. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1748-1759.	1.1	5
49	Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4058-4066.	1.1	5
50	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. <i>Journal of Chemical Physics</i> , 2021, 155, 094302.	1.2	4
51	Density functional theory based generalized effective fragment potential method. <i>Journal of Chemical Physics</i> , 2014, 140, 244101.	1.2	3
52	Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11234-11248.	1.3	1