Kiet A Nguyen

List of Publications by Year
in descending order

52	21,156	186265	175258
papers	citations	28 h-index	52 g-index

52	52	52	15561
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	3.3	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.	3.0	212
3	Observation and Interpretation of Annulated Porphyrins:Â Studies on the Photophysical Properties ofmeso-Tetraphenylmetalloporphyrins. Journal of Physical Chemistry A, 2003, 107, 11331-11339.	2.5	160
4	A dualâ€level Shepard interpolation method for generating potential energy surfaces for dynamics calculations. Journal of Chemical Physics, 1995, 103, 5522-5530.	3.0	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.	3.1	115
6	TDDFT Study of One- and Two-Photon Absorption Properties:Â Donorâ^Ï€â^'Acceptor Chromophores. Journal of Physical Chemistry B, 2005, 109, 1803-1814.	2.6	101
7	Analysis of Absorption Spectra of Zinc Porphyrin, Zinc meso-Tetraphenylporphyrin, and Halogenated Derivatives. Journal of Physical Chemistry A, 2002, 106, 10285-10293.	2.5	81
8	Reactionâ€path dynamics in curvilinear internal coordinates including torsions. Journal of Chemical Physics, 1996, 104, 6491-6496.	3.0	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.	3.0	68
10	A density functional theory study of phosphorescence and tripletâ€“triplet absorption for nonlinear absorption chromophores. Journal of Chemical Physics, 2002, 117, 7128-7136.	3.0	67
11	Calculation of two-photon absorption spectra of donor-Ï€-acceptor compounds in solution using quadratic response time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 094103.	3.0	63
12	The Inversion of Bicyclobutane and Bicyclodiazoxane. Journal of the American Chemical Society, 1994, 116, 9241-9249.	13.7	58
13	Isomerization Of Bicyclo[1.1.0]butane to Butadiene. Journal of the American Chemical Society, 1995, 117, 3835-3847.	13.7	55
14	Effect of hydration and dimerization of the formamidine rearrangement. Journal of the American Chemical Society, 1991, 113, 1596-1600.	13.7	51
15	Triplet Excited States of Free-Base Porphin and Its Î²-Octahalogenated Derivativesâ€. Journal of Physical Chemistry A, 2000, 104, 4748-4754.	2.5	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.	5.3	51
17	Stabilization of .beta. positive charge by silicon, germanium, or tin. Organometallics, 1991, 10, 2798-2803.	2.3	50
18	Jahnâ€“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.	3.0	50

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19	The structure and bonding in group IV [1.1.1]Propellanes. Polyhedron, 1991, 10, 1247-1264.	2.2	48
20	Calculation of One- and Two-Photon Absorption Spectra of Thiolated Gold Nanoclusters using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2010, 6, 2809-2821.	5.3	47
21	The performance and relationship among range-separated schemes for density functional theory. Journal of Chemical Physics, 2011, 135, 074109.	3.0	43
22	Effects of Conjugation in Length and Dimension on Spectroscopic Properties of Fluorene-Based Chromophores from Experiment and Theory. Journal of Physical Chemistry A, 2006, 110, 13172-13182.	2.5	42
23	Structures and bonding of Group IVA sulfur and oxygen propellane derivatives. Journal of the American Chemical Society, 1991, 113, 7924-7929.	13.7	40
24	Ground and Triplet Excited Structures and Spectroscopic Properties of Halogenated Zincmeso-Tetraphenylporphyrin. Journal of Physical Chemistry A, 1999, 103, 9378-9382.	2.5	37
25	Analysis of nonlinear optical properties in donorâ€“acceptor materials. Journal of Chemical Physics, 2014, 140, 184308.	3.0	32
26	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. Journal of Physical Chemistry A, 2016, 120, 507-518.	2.5	31
27	Structure, Bonding, and Stability of Small Boronâˆ’Lithium Clusters. Journal of Physical Chemistry A, 1998, 102, 1608-1614.	2.5	29
28	One- and Two-Photon Spectra of Platinum Acetylide Chromophores: A TDDFT Study. Journal of Physical Chemistry A, 2009, 113, 13943-13952.	2.5	28
29	Addition of a Phenyl Phosphinidene Complex to Conjugated Diynes. Organometallics, 1999, 18, 796-799.	2.3	27
30	Calculation of One-Photon and Two-Photon Absorption Spectra of Porphyrins Using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1094-1106.	5.3	27
31	Theoretical studies of spinâ€forbidden radiationless decay in polyatomic systems. II. Radiationless decay of aâ€N2O2. Journal of Chemical Physics, 1993, 98, 3845-3849.	3.0	26
32	Analytical energy gradients of Coulombâ€attenuated timeâ€dependent density functional methods for excited states. International Journal of Quantum Chemistry, 2010, 110, 2247-2255.	2.0	22
33	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of N2O2. Journal of Physical Chemistry A, 1997, 101, 4283-4289.	2.5	21
34	Effects of conjugation in length and dimension on two-photon properties of fluorene-based chromophores. Theoretical Chemistry Accounts, 2008, 120, 167-175.	1.4	19
35	Systematic survey of cyclic silicon-oxygen compounds. Journal of the American Chemical Society, 1991, 113, 5998-6001.	13.7	18
36	Photoinduced Hydrogen Atom Transfer of Free-Base Porphin. Journal of Physical Chemistry A, 2000, 104, 4549-4552.	2.5	18

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37	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. Journal of Chemical Physics, 2015, 142, 234305.	3.0	18
38	Stability of Hyperlithiated Borides. Journal of Physical Chemistry A, 1999, 103, 710-715.	2.5	15
39	Ab Initio Study of the Thermal Isomerization of Tricyclo[3.1.0.02,6]hexane to (Z,Z)-1,3-Cyclohexadiene through the (E,Z)-1,3-Cyclohexadiene Intermediate. Journal of Physical Chemistry A, 2003, 107, 198-203.	2.5	14
40	Alternative Mechanisms in Hydrogen Production by Aluminum Anion Clusters. Journal of Chemical Theory and Computation, 2012, 8, 152-161.	5.3	13
41	Systematic Study of Structure, Stability, and Electronic Absorption of Tetrahedral CdSe Clusters with Carboxylate and Amine Ligands. Journal of Physical Chemistry A, 2018, 122, 6704-6712.	2.5	10
42	Theoretical Prediction of Optical Absorption and Emission in Thiolated Gold Clusters. Journal of Physical Chemistry A, 2019, 123, 6472-6481.	2.5	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. Journal of Physical Chemistry A, 2020, 124, 10472-10481.	2.5	9
44	Matrix-infrared spectra of structural isomers of the phosphorus oxysulfide P4S3O. Inorganic Chemistry, 1990, 29, 5096-5100.	4.0	7
45	A Theoretical Investigation of the Structure and Optical Properties of a Silver Cluster in Solid Form and in Solution. Journal of Physical Chemistry A, 2017, 121, 326-333.	2.5	7
46	Computational design of two-photon active organic molecules for infrared responsive materials. Journal of Materials Chemistry C, 2020, 8, 9867-9873.	5.5	7
47	Isomers on the Si2CH4+ Potential Energy Surface. Organometallics, 1996, 15, 5391-5398.	2.3	5
48	Calculations of One- and Two-Photon Absorption Spectra for Molecular Metal Chalcogenide Clusters with Electron-Acceptor Ligands. Journal of Physical Chemistry A, 2017, 121, 1748-1759.	2.5	5
49	Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. Journal of Physical Chemistry A, 2018, 122, 4058-4066.	2.5	5
50	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. Journal of Chemical Physics, 2021, 155, 094302.	3.0	4
51	Density functional theory based generalized effective fragment potential method. Journal of Chemical Physics, 2014, 140, 244101.	3.0	3
52	Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. Physical Chemistry Chemical Physics, 2022, 24, 11234-11248.	2.8	1