Kiet A Nguyen

List of Publications by Year
in descending order

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52	21,156	212478	198040
papers	citations	28 h-index	52 g-index

52	52	52	17301
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. Physical Chemistry Chemical Physics, 2022, 24, 11234-11248.	1.3	1
2	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. Journal of Chemical Physics, 2021, 155, 094302.	1.2	4
3	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.	1.1	9
4	Computational design of two-photon active organic molecules for infrared responsive materials. Journal of Materials Chemistry C, 2020, 8, 9867-9873.	2.7	7
5	Theoretical Prediction of Optical Absorption and Emission in Thiolated Gold Clusters. Journal of Physical Chemistry A, 2019, 123, 6472-6481.	1.1	9
6	Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. Journal of Physical Chemistry A, 2018, 122, 4058-4066.	1.1	5
7	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.	1.1	10
8	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.	1.1	5
9	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.	1.1	7
10	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. Journal of Physical Chemistry A, 2016, 120, 507-518.	1.1	31
11	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. Journal of Chemical Physics, 2015, 142, 234305.	1.2	18
12	Analysis of nonlinear optical properties in donorâ€“acceptor materials. Journal of Chemical Physics, 2014, 140, 184308.	1.2	32
13	Density functional theory based generalized effective fragment potential method. Journal of Chemical Physics, 2014, 140, 244101.	1.2	3
14	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
15	Alternative Mechanisms in Hydrogen Production by Aluminum Anion Clusters. Journal of Chemical Theory and Computation, 2012, 8, 152-161.	2.3	13
16	The performance and relationship among range-separated schemes for density functional theory. Journal of Chemical Physics, 2011, 135, 074109.	1.2	43
17	Analytical energy gradients of Coulombâ€attenuated timeâ€dependent density functional methods for excited states. International Journal of Quantum Chemistry, 2010, 110, 2247-2255.	1.0	22
18	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

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19	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.	2.3	47
20	One- and Two-Photon Spectra of Platinum Acetylide Chromophores: A TDDFT Study. Journal of Physical Chemistry A, 2009, 113, 13943-13952.	1.1	28
21	Effects of conjugation in length and dimension on two-photon properties of fluorene-based chromophores. Theoretical Chemistry Accounts, 2008, 120, 167-175.	0.5	19
22	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.	2.3	27
23	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.	1.1	42
24	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.	1.2	63
25	TDDFT Study of One- and Two-Photon Absorption Properties:Â Donorâ^Ï€â^'Acceptor Chromophores. Journal of Physical Chemistry B, 2005, 109, 1803-1814.	1.2	101
26	Observation and Interpretation of Annulated Porphyrins:Â Studies on the Photophysical Properties ofmeso-Tetraphenylmetalloporphyrins. Journal of Physical Chemistry A, 2003, 107, 11331-11339.	1.1	160
27	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.	1.1	14
28	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.	1.2	50
29	A density functional theory study of phosphorescence and tripletâ€"triplet absorption for nonlinear absorption chromophores. Journal of Chemical Physics, 2002, 117, 7128-7136.	1.2	67
30	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
31	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
32	Triplet Excited States of Free-Base Porphin and Its Î²-Octahalogenated Derivativesâ€. Journal of Physical Chemistry A, 2000, 104, 4748-4754.	1.1	51
33	Photoinduced Hydrogen Atom Transfer of Free-Base Porphin. Journal of Physical Chemistry A, 2000, 104, 4549-4552.	1.1	18
34	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
35	Stability of Hyperlithiated Borides. Journal of Physical Chemistry A, 1999, 103, 710-715.	1.1	15
36	Ground and Triplet Excited Structures and Spectroscopic Properties of Halogenated Zincmeso-Tetraphenylporphyrin. Journal of Physical Chemistry A, 1999, 103, 9378-9382.	1.1	37

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37	Addition of a Phenyl Phosphinidene Complex to Conjugated Diynes. Organometallics, 1999, 18, 796-799.	1.1	27
38	Structure, Bonding, and Stability of Small Boronâ^'Lithium Clusters. Journal of Physical Chemistry A, 1998, 102, 1608-1614.	1.1	29
39	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of N2O2. Journal of Physical Chemistry A, 1997, 101, 4283-4289.	1.1	21
40	Isomers on the Si2CH4+ Potential Energy Surface. Organometallics, 1996, 15, 5391-5398.	1.1	5
41	Reactionâ€path dynamics in curvilinear internal coordinates including torsions. Journal of Chemical Physics, 1996, 104, 6491-6496.	1.2	74
42	A dualâ€level Shepard interpolation method for generating potential energy surfaces for dynamics calculations. Journal of Chemical Physics, 1995, 103, 5522-5530.	1.2	142
43	Isomerization Of Bicyclo[1.1.0]butane to Butadiene. Journal of the American Chemical Society, 1995, 117, 3835-3847.	6.6	55
44	The Inversion of Bicyclobutane and Bicyclodiazoxane. Journal of the American Chemical Society, 1994, 116, 9241-9249.	6.6	58
45	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	1.5	19,020
46	Theoretical studies of spinâ€forbidden radiationless decay in polyatomic systems. II. Radiationless decay of aâ€N2O2. Journal of Chemical Physics, 1993, 98, 3845-3849.	1.2	26
47	Effect of hydration and dimerization of the formamidine rearrangement. Journal of the American Chemical Society, 1991, 113, 1596-1600.	6.6	51
48	Structures and bonding of Group IVA sulfur and oxygen propellane derivatives. Journal of the American Chemical Society, 1991, 113, 7924-7929.	6.6	40
49	Stabilization of .beta. positive charge by silicon, germanium, or tin. Organometallics, 1991, 10, 2798-2803.	1.1	50
50	Systematic survey of cyclic silicon-oxygen compounds. Journal of the American Chemical Society, 1991, 113, 5998-6001.	6.6	18
51	The structure and bonding in group IV [1.1.1]Propellanes. Polyhedron, 1991, 10, 1247-1264.	1.0	48
52	Matrix-infrared spectra of structural isomers of the phosphorus oxysulfide P4S3O. Inorganic Chemistry, 1990, 29, 5096-5100.	1.9	7