

Yongqing

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7673282/publications.pdf>

Version: 2024-02-01

93
papers

1,460
citations

304743

22
h-index

395702

33
g-index

94
all docs

94
docs citations

94
times ranked

1227
citing authors

#	ARTICLE	IF	CITATIONS
1	The Excess Electron in a Boron Nitride Nanotube: Pyramidal NBO Charge Distribution and Remarkable First Hyperpolarizability. <i>Chemistry - A European Journal</i> , 2012, 18, 11350-11355.	3.3	87
2	Redox control of ferrocene-based complexes with systematically extended π -conjugated connectors: switchable and tailorable second order nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4900.	2.8	69
3	Second-Order Nonlinear Optical Response of Electron Donor-Acceptor Hybrids Formed between Corannulene and Metallofullerenes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24965-24975.	3.1	60
4	Impact of Redox Stimuli on Ferrocene-Buckybowl Complexes: Switchable Optoelectronic and Nonlinear Optical Properties. <i>Organometallics</i> , 2014, 33, 3341-3352.	2.3	46
5	Theoretical design and characterization of pyridalthiadiazole-based chromophores with fast charge transfer at donor/acceptor interface toward small molecule organic photovoltaics. <i>RSC Advances</i> , 2015, 5, 29401-29411.	3.6	46
6	Quantum Chemical Study of Redox-Switchable Second-Order Nonlinear Optical Responses of D π A System BNbpy and Metal Pt(II) Chelate Complex. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13564-13572.	2.5	44
7	Formation Mechanisms, Structure, Solution Behavior, and Reactivity of Aminodiborane. <i>Journal of the American Chemical Society</i> , 2015, 137, 12406-12414.	13.7	42
8	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 81, 25-31.	2.4	42
9	Ferrocene/fullerene hybrids showing large second-order nonlinear optical activities: impact of the cage unit size. <i>Dalton Transactions</i> , 2015, 44, 10078-10088.	3.3	38
10	Constructing nanosized polyanions with diverse structures by the self-assembly of W/Nb mixed-addendum polyoxometalate and lanthanide ion. <i>CrystEngComm</i> , 2012, 14, 1397-1404.	2.6	37
11	Large Nonlinear Optical Responses of Dimers Bearing a Donor and Acceptor: Long, Intradimer Multicenter Bonding. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28746-28756.	3.1	37
12	A thorough understanding of the nonlinear optical properties of BODIPY/carborane/diketopyrrolopyrrole hybrid chromophores: module contribution, linear combination, one-/two-dimensional difference and carborane's arrangement. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7531-7547.	5.5	36
13	Spirooxazine molecular switches with nonlinear optical responses as selective cation sensors. <i>RSC Advances</i> , 2017, 7, 642-650.	3.6	35
14	Strategy for Enhancing Second-Order Nonlinear Optical Properties of the Pt(II) Dithienylethene Complexes: Substituent Effect, π -Conjugated Influence, and Photoisomerization Switch. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12497-12510.	2.5	34
15	Theoretical Study on the Relationship between Spin Multiplicity Effects and Nonlinear Optical Properties of the Pyrrole Radical (C ₄ H ₄ N \dot{A}). <i>Journal of Physical Chemistry A</i> , 2008, 112, 83-88.	2.5	32
16	Intramolecular photo-induced electron transfer in nonlinear optical chromophores: Fullerene (C ₆₀) derivatives. <i>Organic Electronics</i> , 2016, 33, 290-299.	2.6	27
17	Effective Impact of Dielectric Constant on Thermally Activated Delayed Fluorescence and Nonlinear Optical Properties: Through-Bond-/Space Charge Transfer Architectures. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18850-18859.	3.1	27
18	Self-assembly of metal-organic frameworks based on N-donor ligand and flexible tricarboxylic acids with different angular characters. <i>CrystEngComm</i> , 2013, 15, 8214.	2.6	26

#	ARTICLE	IF	CITATIONS
19	BN Segment Doped Effect on the First Hyperpolarizability of Heteronanotubes: Focused on an Effective Connecting Pattern. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10039-10044.	3.1	26
20	Third order NLO properties of corannulene and its Li-doped dimers: effect of concave and convex structures. <i>RSC Advances</i> , 2015, 5, 79783-79791.	3.6	24
21	Third-Order Nonlinear Optical Properties of Endohedral Fullerene (H ₂) ₂ @C ₇₀ and (H ₂ O) ₂ @C ₇₀ Accompanied by the Prospective of Novel (HF) ₂ @C ₇₀ . <i>Journal of Physical Chemistry C</i> , 2018, 122, 6835-6845.	3.1	24
22	Enhancement of second-order nonlinear optical response in boron nitride nanocone: Li-doped effect. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 48, 28-35.	2.4	23
23	Improving the NLO response of bis-cyclometalated iridium(III) complexes by modifying ligands: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2018, 869, 18-25.	1.8	23
24	Structural, Electronic, Stability, and Optical Properties of CsPb _{1-x} SnxI _{Br} 2 Perovskites: A First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20476-20487.	3.1	23
25	A structure-property interplay between the width and height of cages and the static third order nonlinear optical responses for fullerenes: applying gamma density analysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2322-2331.	2.8	20
26	Multinuclear Staircase Oligomers Based on the (Et ₂ C ₂ B ₄ H ₄)Fe(⁶ -C ₆ H ₆) Sandwich Unit: Quantitative Tailorable and Redox Switchable Nonlinear Optics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16470-16480.	3.1	20
27	The novel link between planar m ⁺ bius aromatic and third order nonlinear optical properties of metal-bridged polycyclic complexes. <i>Scientific Reports</i> , 2017, 7, 10182.	3.3	19
28	Planar Octagonal Tetranuclear Cobaltacarborane Macrocyclic [(⁵ -C ₅ Me ₅)Co(2,3-Et ₂ C ₂ B ₄ H ₃ -5-C ₅ H ₅) ₂] ₂ for 2D Nonlinear Optics: Ultra-High-Response and Multistate Controlled Cubic NLO Switch. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28462-28474.	3.1	19
29	Regulation of the Molecular Architectures on Second-Order Nonlinear Optical Response and Thermally Activated Delayed Fluorescence Property: Homoconjugation and Twisted Donor-Acceptor. <i>Journal of Physical Chemistry C</i> , 2020, 124, 921-931.	3.1	19
30	Second-order NLO properties of bis-cyclometalated iridium(III) complexes: Substituent effect and redox switch. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 131-138.	2.4	18
31	Efficient enhancement of second order nonlinear optical response by complexing metal cations in conjugated 7-substituted coumarin. <i>Organic Electronics</i> , 2017, 47, 152-161.	2.6	17
32	Self-Assembled Donor-Acceptor Chromophores: Evident Layer Effect on the First Hyperpolarizability and Two-Dimensional Charge Transfer Character. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21616-21626.	3.1	17
33	Helical Carbon Segment in Carbon-Boron Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. <i>ChemPlusChem</i> , 2014, 79, 732-736.	2.8	16
34	Second-order nonlinear optical responses of carboranyl-substituted indole/indoline derivatives: impact of different substituents. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 111-118.	2.4	15
35	The structural, electronic, and optical properties of organic-inorganic mixed halide perovskites CH		

#	ARTICLE	IF	CITATIONS
37	Theoretical study on the charge transfer mechanism at donor/acceptor interface: Why TTF/TCNQ is inadaptible to photovoltaics?. <i>Journal of Chemical Physics</i> , 2016, 145, 244705.	3.0	13
38	Second-order NLO responses of two-cavity inorganic electrides $\text{Li}_{n-1}\text{B}_{20}\text{H}_{26}$ ($n = 1, 2$): evolutions with increasing excess electron number and various B-B connection sites of $\text{B}_{20}\text{H}_{26}$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2557-2566.	2.8	13
39	The second-order nonlinear optical property of hydrazones-based photochromic complexes: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 327, 114882.	4.9	13
40	Structural and electronic properties of alkali metal peroxides at high pressures. <i>RSC Advances</i> , 2015, 5, 104337-104342.	3.6	12
41	A cation-selective and anion-controlled benzothiazolyl-attached macrocycle for NLO-based cation detection: variational first hyperpolarizabilities. <i>New Journal of Chemistry</i> , 2018, 42, 6091-6100.	2.8	12
42	Optical properties of photovoltaic materials: Organic-inorganic mixed halide perovskites $\text{CH}_3\text{NH}_3\text{Pb}(\text{I}_{1-y}\text{X}_y)_3$ ($\text{X} = \text{Cl}, \text{Br}$). <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 1-8.	2.5	12
43	Redox-triggered switch based on platinum(II) acetylacetonate complexes bearing an isomeric donor-acceptor conjugation ligand shows a high second-order nonlinear optical response. <i>New Journal of Chemistry</i> , 2019, 43, 11263-11274.	2.8	12
44	Impact of the dielectric constant on the first hyperpolarizabilities and the Singlet-Triplet gap in T- and V-Shaped donor-acceptor-donor molecules. <i>Organic Electronics</i> , 2019, 70, 193-204.	2.6	12
45	Tuning of Second-Order Nonlinear Optical Properties Based on [2.2]Paracyclophanes Isomer: the Relative Configuration and Polarizable Environment. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21692-21701.	3.1	12
46	Strong Boron-Carbon Bonding Interaction Drives CO_2 Reduction to Ethanol over the Boron-Doped Cu(111) Surface: An Insight from the First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 572-582.	3.1	12
47	Interlayer charge-transfer in impacting the second hyperpolarizabilities: Radical and cation species of hexathiophenalenylium and its nitro dimers. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 55, 33-40.	2.4	11
48	Second-Order Nonlinear Optical Properties of Carboranylated Square-Planar Pt(II) Zwitterionic Complexes: One-/Two-Dimensional Difference and Substituent Effect. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9330-9340.	2.5	11
49	Effect of π -conjugate units on the ferrocene-based complexes: Switchable second order nonlinear optics controlled by redox stimuli. <i>Dyes and Pigments</i> , 2016, 126, 29-37.	3.7	11
50	The inspiration and challenge for through-space charge transfer architecture: from thermally activated delayed fluorescence to non-linear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15881-15898.	2.8	11
51	New Structure-Nonlinear Optical Property Correlation in Russian Doll-Complexes Formed by Nested Pd(II) Nanorings. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12655-12664.	3.1	10
52	The effect of heterocyclic π bridges on second order nonlinear optical properties of compounds formed between ferrocenyl and corannulene. <i>RSC Advances</i> , 2016, 6, 97063-97069.	3.6	9
53	DFT/TDDFT, NPA, and AIM-based study of the molecular switching properties of photocyclization and metallochromism of the DAE complexes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	9
54	Application of Multifunctional X-Doped Sumanene ($\text{X} = \text{Si}, \text{Ge}, \text{O}, \text{S}$ and Se) for Concave-Convex Supramolecular Assembly with C_{60} and Their Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27811-27822.	3.1	9

#	ARTICLE	IF	CITATIONS
73	Two M(II)-1,5-NDS- <i>dafo</i> supramolecular architectures (M = Cu, Cd): syntheses, structures, and photoluminescence properties. <i>Journal of Coordination Chemistry</i> , 2013, 66, 2702-2711.	2.2	3
74	Probe the accumulation modes of the Au ⁺ C ₂₂ H ₁₄ dimer on the structure and NLO properties. <i>Molecular Physics</i> , 2014, 112, 1918-1923.	1.7	3
75	Theoretical investigation on second-order nonlinear optical properties of ruthenium alkynyl ⁺ dihydroazulene/vinylheptafulvene complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 363-371.	2.4	3
76	The effect of conformational dependent properties of radical cations on poly(N,N-dimethylaniline). <i>Macromolecular Chemistry and Physics</i> , 2000, 201, 1774-1779.	2.2	2
77	Theoretical study on second-order nonlinear optical properties of spin crossover Fe(III) phenolate ⁺ pyridyl Schiff base complexes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1863-1870.	2.0	2
78	Theoretical investigation on structures, electronic spectra and nonlinear optical properties of gold compounds [X ⁺ Au(PMe ₃) ₂]. <i>Science China Chemistry</i> , 2010, 53, 1149-1154.	8.2	2
79	Structures and properties of metal-free and magnesium tetrathieno[2,3-b]porphyrazine investigated using density functional theory. <i>Science China Chemistry</i> , 2010, 53, 1746-1753.	8.2	2
80	Theoretical study on stability and nonlinear optical properties of tetrahydropyrrole diradical and its isoelectronic systems in different electronic states. <i>Science China Chemistry</i> , 2011, 54, 1086-1093.	8.2	2
81	Syntheses, structures, and photoluminescence properties of Zn(II)/Cd(II) supramolecular architectures based on 1,5-naphthalenedisulfonate and 1,10-phenanthroline ligands. <i>Monatshefte für Chemie</i> , 2013, 144, 1507-1512.	1.8	2
82	THEORETICAL INVESTIGATION ON PHOTOISOMERIZATION SWITCHABLE SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF β -SHAPED DIARYLETHENE DERIVATIVES. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350029.	1.8	2
83	The second-order NLO property of a photoswitchable heteroditopic ion-pair receptor based on 2-pyridyl acylhydrazone linking with 2,6-pyridine bisamide: The impacts of metal cations and anions. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107652.	2.4	2
84	Regulating the NLO response of anthraquinone-supported thiourea-linked crown ether macrocycle by introducing metal cations: A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050017.	1.8	2
85	Structural, electrical, optical properties and stability of Cs ₂ InBr ₅ -yXy ⁺ H ₂ O (X = Cl, I, y = 0, 1, 2, 3, 4, 5) perovskites: the first principles investigation. <i>Thin Solid Films</i> , 2021, 733, 138805.	1.8	2
86	The influence of M ⁺ M attraction on nonlinear optical properties of (XMPH ₃) ₂ (X = F, Cl; and M = Au, Ag and Cu): A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 865-873.	2.0	1
87	Quantum chemical studies on tuning the second-order nonlinear optical molecular switching of triarylborane derivatives. <i>Science Bulletin</i> , 2012, 57, 1772-1780.	1.7	1
88	Second-order nonlinear optical response of phenyl-substituted cationic BIS-cyclometalated iridium(III) complexes: Effect of different position. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850033.	1.8	1
89	DFT study of effect of substituents on second-order NLO response of novel BODIPY dyes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	1
90	Quantum chemical study on ferromagnetic property on the N,N-dimethylaniline dimer radical cation. <i>International Journal of Quantum Chemistry</i> , 2002, 89, 484-488.	2.0	0

#	ARTICLE	IF	CITATIONS
91	Inside Cover: Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in Möbius Cyclacenes: New Insight into the Localized π Electrons (ChemPhysChem 9/2012). ChemPhysChem, 2012, 13, 2222-2222.	2.1	0
92	Switchable second-order nonlinear optical response of platinum-sensitized dithienylethenes. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950022.	1.8	0
93	Electronic and Optical Properties of C ₄ N ₂ H ₁₄ -Based Lead-Less Halide Perovskites Investigated by First Principles. Journal of Physical Chemistry C, 2021, 125, 19445-19454.	3.1	0