

# 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	Electroreduction of N <sub>2</sub> to NH <sub>3</sub> catalyzed by a Mn/Re(111) single-atom alloy catalyst with high activity and selectivity: a new insight from a first-principles study. <i>Catalysis Science and Technology</i> , 2022, 12, 4074-4085.	4.1	6
2	Theoretical investigation of electronic structures, second-order NLO responses of cyclometalated Ir(III) and Rh(III) counterpart complexes: effect of metal centers. <i>New Journal of Chemistry</i> , 2022, 46, 10652-10661.	2.8	7
3	A computational study on second-order nonlinear optical properties based on bis-cyclometalated Ir(III) complexes: redox and substituent effects. <i>New Journal of Chemistry</i> , 2021, 45, 10725-10734.	2.8	8
4	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
5	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
6	Electronic and Optical Properties of C <sub>4</sub> N <sub>2</sub> H <sub>14</sub> -Based Lead-Less Halide Perovskites Investigated by First Principles. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19445-19454.	3.1	0
7	Structural, electrical, optical properties and stability of Cs <sub>2</sub> InBr <sub>5-y</sub> Xy·H <sub>2</sub> 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
8	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
9	Strong Boron-Carbon Bonding Interaction Drives CO <sub>2</sub> 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
10	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
11	Novel cyclic and linearizing cyclic Pd(II) nano-hoop-based coordination complexes achieving nonlinear optical activity transparency trade-off optimization. <i>Organic Electronics</i> , 2020, 78, 105564.	2.6	5
12	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
13	Second-order NLO properties of bis-cyclometalated iridium(III) complexes with $\beta^2$ -diketiminate ancillary ligand: Substituent and redox effect. <i>Inorganica Chimica Acta</i> , 2020, 511, 119835.	2.4	4
14	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
15	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
16	New Structure-Nonlinear Optical Property Correlation in $\pi$ -Russian Doll-Complexes Formed by Nested Pd(II) Nanorings. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12655-12664.	3.1	10
17	Structural, Electronic, Stability, and Optical Properties of CsPb <sub>1-x</sub> Sn <sub>x</sub> Br <sub>2</sub> Perovskites: A First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20476-20487.	3.1	23
18	Application of Multifunctional X-Doped Sumanene (X= Si, Ge, O, S and Se) for Concave-Convex Supramolecular Assembly with C <sub>60</sub> and Their Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27811-27822.	3.1	9

#	ARTICLE	IF	CITATIONS
19	Switchable second-order nonlinear optical response of platinum-sensitized dithienylethenes. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950022.	1.8	0
20	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
21	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
22	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
23	Theoretical exploration of second-order nonlinear optical properties of mono- and bimetallic Pt(II) dithienylcyclopentene complexes: Ligands and photoisomerization effect. <i>Journal of Organometallic Chemistry</i> , 2019, 888, 29-36.	1.8	8
24	DFT Studies on Second-order Nonlinear Optical Response of Ir(C <sup>N</sup> ) <sub>2</sub> (pic) Complexes. <i>Chemical Research in Chinese Universities</i> , 2019, 35, 333-339.	2.6	4
25	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
26	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
27	Third-Order Nonlinear Optical Properties of Endohedral Fullerene (H <sub>2</sub> ) <sub>2</sub> @C <sub>70</sub> and (H <sub>2</sub> O) <sub>2</sub> @C <sub>70</sub> Accompanied by the Prospective of Novel (HF) <sub>2</sub> @C <sub>70</sub> . <i>Journal of Physical Chemistry C</i> , 2018, 122, 6835-6845.	3.1	24
28	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
29	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
30	Optical properties of photovoltaic materials: Organic-inorganic mixed halide perovskites CH <sub>3</sub> NH <sub>3</sub> Pb(I <sub>1-y</sub> X <sub>y</sub> ) <sub>3</sub> (X = Cl, Br). <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 1-8.	2.5	12
31	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
32	The structural, electronic, and optical properties of organic-inorganic mixed halide perovskites CH		

#	ARTICLE	IF	CITATIONS
37	Second-order NLO responses of two-cavity inorganic electrides $\text{Li}_n @ \text{B}_{20}\text{H}_{26}$ ( $n = 1, 2$ ): evolutions with increasing excess electron number and various B connection sites of $\text{B}_{20}\text{H}_{26}$ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2557-2566.	2.8	13
38	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
39	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
40	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
41	The novel link between planar m <sup>3</sup> aromatic and third order nonlinear optical properties of metal-bridged polycyclic complexes. <i>Scientific Reports</i> , 2017, 7, 10182.	3.3	19
42	Multinuclear Staircase-Oligomers Based on the $(\text{Et}_2\text{C}_2\text{B}_4\text{H}_4)\text{Fe}(\text{I}_6\text{-C}_6\text{H}_6)$ Sandwich Unit: Quantitative Tailorable and Redox Switchable Nonlinear Optics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16470-16480.	3.1	20
43	Planar Octagonal Tetranuclear Cobaltacarborane Macrocycle $[(\text{I}_5\text{-C}_5\text{Me}_5)\text{Co}(2,3\text{-Et}_2\text{C}_2\text{B}_4\text{H}_3)]$ 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
44	Structural transitions and electronic properties of sodium superoxide at high pressures. <i>RSC Advances</i> , 2016, 6, 67910-67915.	3.6	5
45	Theoretical study on the charge transfer mechanism at donor/acceptor interface: Why TTF/TCNQ is inadaptable to photovoltaics?. <i>Journal of Chemical Physics</i> , 2016, 145, 244705.	3.0	13
46	Intramolecular photo-induced electron transfer in nonlinear optical chromophores: Fullerene (C60) derivatives. <i>Organic Electronics</i> , 2016, 33, 290-299.	2.6	27
47	Electronic properties of SrFeO <sub>2</sub> doped by Ca and Ba: A first-principles study. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 112-117.	2.5	7
48	The effect of heterocyclic $\eta$ bridges on second order nonlinear optical properties of compounds formed between ferrocenyl and corannuleny. <i>RSC Advances</i> , 2016, 6, 97063-97069.	3.6	9
49	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
50	Second-Order Nonlinear Optical Responses and Concave-Convex Interactions of Size-Selective Fullerenes/Corannulene Recognition Pairs: The Effect of Fullerene Size. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26034-26043.	3.1	8
51	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
52	Electronic properties of polyoxometalate derivatives $[(\text{C}_2\text{B}_9\text{H}_{11})\text{M}'\text{M}_5\text{O}_{18}]^{n-}$ ( $\text{M}' = \text{Tl}^{\text{IV}}$ , $\text{M} = \text{V}^{\text{VI}}$ ), <i>Tj ETQq 0 0 rgBT /Overlock 10 Tf 50 137 T</i>		
53	Effect of $\eta$ -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
54	Ion- $\eta$ interaction in impacting the nonlinear optical properties of ion-buckybowl complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 64, 139-146.	2.4	5

#	ARTICLE	IF	CITATIONS
55	Structural and electronic properties of alkali metal peroxides at high pressures. <i>RSC Advances</i> , 2015, 5, 104337-104342.	3.6	12
56	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
57	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
58	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
59	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
60	Formation Mechanisms, Structure, Solution Behavior, and Reactivity of Aminodiborane. <i>Journal of the American Chemical Society</i> , 2015, 137, 12406-12414.	13.7	42
61	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
62	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
63	Helical Carbon Segment in Carbon-Boron-Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. <i>ChemPlusChem</i> , 2014, 79, 732-736.	2.8	16
64	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
65	Probe the accumulation modes of the Au-C <sub>22</sub> H <sub>14</sub> dimer on the structure and NLO properties. <i>Molecular Physics</i> , 2014, 112, 1918-1923.	1.7	3
66	Redox control of ferrocene-based complexes with systematically extended $\pi$ -conjugated connectors: switchable and tailorable second order nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4900.	2.8	69
67	Impact of Redox Stimuli on Ferrocene-Buckybowl Complexes: Switchable Optoelectronic and Nonlinear Optical Properties. <i>Organometallics</i> , 2014, 33, 3341-3352.	2.3	46
68	Mechanistic insight into the second-order nonlinear optical properties of Ru-coordinated DTE complexes: Photoisomerization, redox, and protonation switches. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 100-106.	1.8	8
69	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
70	Strategy for Enhancing Second-Order Nonlinear Optical Properties of the Pt(II) Dithienylethene Complexes: Substituent Effect, $\pi$ -Conjugated Influence, and Photoisomerization Switch. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12497-12510.	2.5	34
71	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
72	Two M(II)-1,5-NDS-dafo supramolecular architectures (M = Cu, Cd): syntheses, structures, and photoluminescence properties. <i>Journal of Coordination Chemistry</i> , 2013, 66, 2702-2711.	2.2	3

#	ARTICLE	IF	CITATIONS
73	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
74	THEORETICAL INVESTIGATION ON PHOTOISOMERIZATION SWITCHABLE SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF $\beta$ -SHAPED DIARYLETHENE DERIVATIVES. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350029.	1.8	2
75	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
76	Second-order nonlinear optical responses switching of $N^{\wedge}S^{\wedge}N$ ruthenium carboxylate complexes with proton-electron transfer. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 779-788.	2.0	6
77	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
78	Inside Cover: Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in Möbius Cyclacenes: New Insight into the Localized $\pi$ Electrons ( <i>ChemPhysChem</i> 9/2012). <i>ChemPhysChem</i> , 2012, 13, 2222-2222.	2.1	0
79	Theoretical study on second-order nonlinear optical properties of 1,10-phenanthroline Ru(II) complexes. <i>Science China Chemistry</i> , 2012, 55, 1421-1427.	8.2	5
80	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
81	Quantum Chemical Study of Redox-Switchable Second-Order Nonlinear Optical Responses of $D_{3h}$ System BNbp <sub>3</sub> and Metal Pt(II) Chelate Complex. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13564-13572.	2.5	44
82	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
83	DFT study on the second-order nonlinear optical property of 12-vertex close-carborane derivatives. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1039-1047.	2.0	13
84	The influence of $M \cdots M$ attraction on nonlinear optical properties of $(XMPH)_3$ (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
85	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
86	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
87	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
88	Theoretical studies on electronic spectra and second-order nonlinear optical properties of barbituric acid derivatives substituted with schiff base. <i>Chinese Journal of Chemistry</i> , 2010, 22, 425-429.	4.9	3
89	DFT study on second-order nonlinear optical properties of Pt(II) complexes with different chromophores. <i>Science in China Series B: Chemistry</i> , 2009, 52, 144-152.	0.8	5
90	Theoretical Study on the Relationship between Spin Multiplicity Effects and Nonlinear Optical Properties of the Pyrrole Radical (C <sub>4</sub> H <sub>4</sub> N $\dot{A}$ ). <i>Journal of Physical Chemistry A</i> , 2008, 112, 83-88.	2.5	32

#	ARTICLE	IF	CITATIONS
91	Structure and second-order NLO property of the molecules bridged through n-vertex bis-substituted carborane (n=5, 6, 7). Science Bulletin, 2007, 52, 2326-2330.	1.7	7
92	Quantum chemical study on ferromagnetic property on the N,N-dimethylaniline dimer radical cation. International Journal of Quantum Chemistry, 2002, 89, 484-488.	2.0	0
93	The effect of conformational dependent properties of radical cations on poly(N,N-dimethylaniline). Macromolecular Chemistry and Physics, 2000, 201, 1774-1779.	2.2	2