

Shilie Pan

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Finding the Next Deep-Ultraviolet Nonlinear Optical Material: $\text{NH}_4\text{B}_4\text{O}_6\text{F}$. <i>Journal of the American Chemical Society</i> , 2017, 139, 10645-10648.	6.6	889
2	Fluorooxoborates: Beryllium-Free Deep-Ultraviolet Nonlinear Optical Materials without Layered Growth. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3916-3919.	7.2	674
3	$\text{CsB}_4\text{O}_6\text{F}$: A Congruent-Melting Deep-Ultraviolet Nonlinear Optical Material by Combining Superior Functional Units. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14119-14123.	7.2	654
4	$\text{K}_3\text{B}_6\text{O}_{10}\text{Cl}$: A New Structure Analogous to Perovskite with a Large Second Harmonic Generation Response and Deep UV Absorption Edge. <i>Journal of the American Chemical Society</i> , 2011, 133, 7786-7790.	6.6	617
5	$\text{SrB}_5\text{O}_7\text{F}_3$ Functionalized with $[\text{B}_5\text{O}_9\text{F}_3]^{6-}$ Chromophores: Accelerating the Rational Design of Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6095-6099.	7.2	581
6	Designing a Deep-Ultraviolet Nonlinear Optical Material with a Large Second Harmonic Generation Response. <i>Journal of the American Chemical Society</i> , 2013, 135, 4215-4218.	6.6	542
7	Borates: A Rich Source for Optical Materials. <i>Chemical Reviews</i> , 2021, 121, 1130-1202.	23.0	534
8	Cation-Tuned Synthesis of Fluorooxoborates: Towards Optimal Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 2150-2154.	7.2	527
9	Polar Fluorooxoborate, $\text{NaB}_4\text{O}_6\text{F}$: A Promising Material for Ionic Conduction and Nonlinear Optics. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6577-6581.	7.2	368
10	Designing an Excellent Deep-Ultraviolet Birefringent Material for Light Polarization. <i>Journal of the American Chemical Society</i> , 2018, 140, 16311-16319.	6.6	350
11	Targeting the Next Generation of Deep-Ultraviolet Nonlinear Optical Materials: Expanding from Borates to Borate Fluorides to Fluorooxoborates. <i>Accounts of Chemical Research</i> , 2019, 52, 791-801.	7.6	315
12	$\text{Ba}_3\text{Mg}_3(\text{BO}_3)_3\text{F}_3$ polymorphs with reversible phase transition and high performances as ultraviolet nonlinear optical materials. <i>Nature Communications</i> , 2018, 9, 3089.	5.8	314
13	$\text{Cs}_3\text{Zn}_6\text{B}_9\text{O}_{21}$: A Chemically Benign Member of the KBBF Family Exhibiting the Largest Second Harmonic Generation Response. <i>Journal of the American Chemical Society</i> , 2014, 136, 1264-1267.	6.6	310
14	A New Deep-Ultraviolet Transparent Orthophosphate LiCs_2PO_4 with Large Second Harmonic Generation Response. <i>Journal of the American Chemical Society</i> , 2016, 138, 9101-9104.	6.6	307
15	Recent development of metal borate halides: Crystal chemistry and application in second-order NLO materials. <i>Coordination Chemistry Reviews</i> , 2016, 323, 15-35.	9.5	272
16	$\text{Na}_2\text{ZnGe}_2\text{S}_6$: A New Infrared Nonlinear Optical Material with Good Balance between Large Second-Harmonic Generation Response and High Laser Damage Threshold. <i>Journal of the American Chemical Society</i> , 2016, 138, 7422-7428.	6.6	259
17	$\text{Pb}_2\text{Ba}_3(\text{BO}_3)_3\text{Cl}$: A Material with Large SHG Enhancement Activated by Pb-Chelated BO_3 Groups. <i>Journal of the American Chemical Society</i> , 2015, 137, 9417-9422.	6.6	255
18	$\text{Cs}_2\text{B}_4\text{SiO}_9$: A Deep-Ultraviolet Nonlinear Optical Crystal. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3406-3410.	7.2	249

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19	Synthesis, Crystal Structure, and Nonlinear Optical Properties of Li ₆ CuB ₄ O ₁₀ : A Congruently Melting Compound with Isolated [CuB ₄ O ₁₀] ₆ -Units. <i>Journal of the American Chemical Society</i> , 2006, 128, 11631-11634.	6.6	219
20	Emergent Deep-Ultraviolet Nonlinear Optical Candidates. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20302-20317.	7.2	203
21	New Compressed Chalcopyrite-like Li ₂ BaM ^{IV} Q ₄ (M ^{IV} = Tl, Pb, Bi, Sb, Sn, Te, Se, S, Ge, Si, C). <i>Journal of the American Chemical Society</i> , 2017, 139, 14885-14888.	6.6	201
22	NH ₄ Be ₂ BO ₃ F ₂ and Be ₂ BO ₃ F ₂ : Overcoming the Layering Habit in KBe ₂ BO ₃ F ₂ for the Next-Generation Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8968-8972.	7.2	200
23	Expanding Frontiers of Ultraviolet Nonlinear Optical Materials with Fluorophosphates. <i>Chemistry of Materials</i> , 2018, 30, 5397-5403.	3.2	193
24	Chemical Cosubstitution-Oriented Design of Rare-Earth Borates as Potential Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , 2017, 139, 18397-18405.	6.6	187
25	Pb ₁₇ O ₈ Cl ₁₈ : A Promising IR Nonlinear Optical Material with Large Laser Damage Threshold Synthesized in an Open System. <i>Journal of the American Chemical Society</i> , 2015, 137, 8360-8363.	6.6	181
26	A novel deep UV nonlinear optical crystal Ba ₃ B ₆ O ₁₁ F ₂ , with a new fundamental building block, B ₆ O ₁₄ group. <i>Journal of Materials Chemistry</i> , 2012, 22, 9665.	6.7	177
27	Rational Design via Synergistic Combination Leads to an Outstanding Deep-Ultraviolet Birefringent Li ₂ Na ₂ B ₂ O ₅ Material with an Unvalued B ₂ O ₅ Functional Gene. <i>Journal of the American Chemical Society</i> , 2019, 141, 3258-3264.	6.6	177
28	Na ₂ BaMQ ₄ (M=Ge, Sn; Q=S, Se): Infrared Nonlinear Optical Materials with Excellent Performances and that Undergo Structural Transformations. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6713-6715.	7.2	172
29	Sn ₂ B ₅ O ₉ Cl: A Material with Large Birefringence Enhancement Activated Prepared via Alkaline-Earth Metal Substitution by Tin. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17675-17678.	7.2	171
30	CsB ₄ O ₆ F: A Congruently Melting Deep-Ultraviolet Nonlinear Optical Material by Combining Superior Functional Units. <i>Angewandte Chemie</i> , 2017, 129, 14307-14311.	1.6	166
31	Enhancing optical anisotropy of crystals by optimizing bonding electron distribution in anionic groups. <i>Chemical Communications</i> , 2017, 53, 2818-2821.	2.2	155
32	Growth, Structure, and Properties of Single Crystals of SrBPO ₅ . <i>Chemistry of Materials</i> , 2003, 15, 2218-2221.	3.2	154
33	CaB ₅ O ₇ F ₃ : A Beryllium-Free Alkaline-Earth Fluorooxoborate Exhibiting Excellent Nonlinear Optical Performances. <i>Inorganic Chemistry</i> , 2018, 57, 4820-4823.	1.9	136
34	Cation-Tuned Synthesis of Fluorooxoborates: Towards Optimal Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie</i> , 2018, 130, 2172-2176.	1.6	131
35	Li ₄ MgGe ₂ S ₇ : The First Alkali and Alkaline-Earth Diamond-Like Infrared Nonlinear Optical Material with Exceptional Large Band Gap. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24131-24136.	7.2	130
36	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , 2018, 140, 10726-10733.	6.6	127

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37	Simulated pressure-induced blue-shift of phase-matching region and nonlinear optical mechanism for $K_3B_6O_{10}X$ ($X = \text{Cl, Br}$). <i>Applied Physics Letters</i> , 2015, 106, .	1.5	121
38	Strong Nonlinearity Induced by Coaxial Alignment of Polar Chain and Dense $[BO_3]_3$ Units in $CaZn_2(BO_3)_2$. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	116
39	Potential optical functional crystals with large birefringence: Recent advances and future prospects. <i>Coordination Chemistry Reviews</i> , 2022, 459, 214380.	9.5	114
40	$Bi_3OF_3(IO_3)_4$: Metal Oxyiodate Fluoride Featuring a Carbon-Nanotube-like Topological Structure with Large Second Harmonic Generation Response. <i>Chemistry of Materials</i> , 2017, 29, 945-949.	3.2	112
41	Discovery of First Magnesium Fluorooxoborate with Stable Fluorine Terminated Framework for Deep-UV Nonlinear Optical Application. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 14650-14656.	7.2	109
42	A new congruent-melting oxyborate, $Pb_4O(BO_3)_2$ with optimally aligned BO_3 triangles adopting layered-type arrangement. <i>Journal of Materials Chemistry</i> , 2012, 22, 2105-2110.	6.7	108
43	$SrB_5O_7F_3$ Functionalized with $[B_5O_9F_3]^{6-}$ Chromophores: Accelerating the Rational Design of Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie</i> , 2018, 130, 6203-6207.	1.6	108
44	$CsAlB_3O_6F$: a beryllium-free deep-ultraviolet nonlinear optical material with enhanced thermal stability. <i>Chemical Science</i> , 2020, 11, 694-698.	3.7	108
45	BaSn_2 : A UV Birefringent Material with Large Birefringence and Easy Crystal Growth. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3540-3544.	7.2	108
46	Growth, Structure, and Optical Properties of a Congruent Melting Oxyborate, $Bi_2ZnOB_2O_6$. <i>Chemistry of Materials</i> , 2009, 21, 2846-2850.	3.2	104
47	Sn_2PO_4I : An Excellent Birefringent Material with Giant Optical Anisotropy in Non-Conjugated Phosphate. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24901-24904.	7.2	101
48	A Novel Nonlinear Optical Crystal $Bi_2ZnOB_2O_6$. <i>Crystal Growth and Design</i> , 2009, 9, 4091-4095.	1.4	99
49	Expanding the chemistry of borates with functional $[BO_2]^-$ anions. <i>Nature Communications</i> , 2021, 12, 2597.	5.8	99
50	A Bulk Boron-Based Photocatalyst for Efficient Dechlorination: $K_3B_6O_{10}Br$. <i>Chemistry of Materials</i> , 2014, 26, 3169-3174.	3.2	97
51	The first quaternary diamond-like semiconductor with 10-membered LiS_4 rings exhibiting excellent nonlinear optical performances. <i>Chemical Communications</i> , 2017, 53, 3010-3013.	2.2	96
52	A congruently melting and deep UV nonlinear optical material: $Li_3Cs_2B_5O_{10}$. <i>Journal of Materials Chemistry</i> , 2011, 21, 2890.	6.7	95
53	Fluorooxoborates: Beryllium-Free Deep-Ultraviolet Nonlinear Optical Materials without Layered Growth. <i>Angewandte Chemie</i> , 2017, 129, 3974-3977.	1.6	94
54	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. <i>Physical Review Letters</i> , 2020, 125, 187402.	2.9	94

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55	Na ₂ B ₆ O ₉ F ₂ : A Fluoroborate with Short Cutoff Edge and Deep-Ultraviolet Birefringent Property Prepared by an Open High-Temperature Solution Method. <i>Inorganic Chemistry</i> , 2017, 56, 344-350.	1.9	92
56	Hydroxyfluorooxoborate Na[B ₃ O ₃ F ₂ (OH) ₂] \cdot ...[B(OH) ₃]: Optimizing the Optical Anisotropy with Heteroanionic Units for Deep Ultraviolet Birefringent Crystals. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20469-20475.	7.2	90
57	KPb ₂ (PO ₃) ₅ : a novel nonlinear optical lead polyphosphate with a short deep-UV cutoff edge. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10630-10637.	2.7	88
58	PbB ₅ O ₇ F ₃ : A High-Performing Short-Wavelength Nonlinear Optical Material. <i>Chemistry of Materials</i> , 2020, 32, 2172-2179.	3.2	88
59	Module-Analysis-Assisted Design of Deep Ultraviolet Fluorooxoborates with Extremely Large Gap and High Structural Stability. <i>Chemistry of Materials</i> , 2019, 31, 2807-2813.	3.2	87
60	UV Nonlinear Optical Crystal Ba ₂ [B ₆ O ₉ (OH) ₄] Featuring Unique Chiral Layers with a New B ₁₈ O ₄₂ Circle Based on BO ₃ and BO ₄ Units. <i>Inorganic Chemistry</i> , 2012, 51, 1852-1858.	1.9	86
61	LiRb ₂ PO ₄ : a new deep-ultraviolet nonlinear optical phosphate with a large SHG response. <i>Journal of Materials Chemistry C</i> , 2017, 5, 269-274.	2.7	84
62	Fluorine-Driven Enhancement of Birefringence in the Fluorooxosulfate: A Deep Evaluation from a Joint Experimental and Computational Study. <i>Advanced Science</i> , 2021, 8, e2003594.	5.6	83
63	Crystal growth and optical properties of a noncentrosymmetric haloid borate, K3B6O10Br. <i>CrystEngComm</i> , 2011, 13, 2899.	1.3	82
64	Deep-Ultraviolet Nonlinear-Optical Material K ₃ Sr ₃ Li ₂ Al ₄ B ₆ O ₂₀ F: Addressing the Structural Instability Problem in KB ₂ BO ₃ F ₂ . <i>Inorganic Chemistry</i> , 2017, 56, 8755-8758.	1.9	82
65	Toward the Enhancement of Critical Performance for Deep-Ultraviolet Frequency-Doubling Crystals Utilizing Covalent Tetrahedra. <i>Accounts of Materials Research</i> , 2021, 2, 282-291.	5.9	82
66	Li4Cs3B7O14: Synthesis, Crystal Structure, and Optical Properties. <i>Inorganic Chemistry</i> , 2011, 50, 2415-2419.	1.9	81
67	Na ₄ B ₈ O ₉ F ₁₀ : A Deep-Ultraviolet Transparent Nonlinear Optical Fluorooxoborate with Unexpected Short Phase-Matching Wavelength Induced by Optimized Chromatic Dispersion. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	80
68	Fluorooxoborates: Ushering in a New Era of Deep Ultraviolet Nonlinear Optical Materials. <i>Chemistry - A European Journal</i> , 2018, 24, 17638-17650.	1.7	79
69	Structure-property survey and computer-assisted screening of mid-infrared nonlinear optical chalcogenides. <i>Coordination Chemistry Reviews</i> , 2020, 421, 213379.	9.5	78
70	Advantageous Units in Antimony Sulfides: Exploration and Design of Infrared Nonlinear Optical Materials. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 26413-26421.	4.0	77
71	Series of Crystals with Giant Optical Anisotropy: A Targeted Strategic Research. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1332-1338.	7.2	77
72	Polar Polymorphism: $\hat{1}^{\pm}$, $\hat{1}^2$, and $\hat{1}^3$ -Pb ₂ Ba ₄ Zn ₄ B ₁₄ O ₃₁ —Synthesis, Characterization, and Nonlinear Optical Properties. <i>Chemistry of Materials</i> , 2015, 27, 4779-4788.	3.2	75

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73	Science China Materials, 2020, 63, 1480-1484.		
74	Synthesis, Structure, and Properties of the Noncentrosymmetric Hydrated Borate $\text{Na}_2\text{B}_5\text{O}_8(\text{OH})\cdot 2\text{H}_2\text{O}$. Inorganic Chemistry, 2009, 48, 7800-7804.	1.9	74
75	$\text{Cs}_4\text{Mo}_5\text{P}_2\text{O}_{22}$: a first Strandberg-type POM with 1D straight chains of polymerized $[\text{Mo}_5\text{P}_2\text{O}_{23}]^{6-}$ units and moderate second harmonic generation response. Chemical Communications, 2013, 49, 306-308.	2.2	74
76	$\text{Hg}_3\text{P}_2\text{S}_8$: A New Promising Infrared Nonlinear Optical Material with a Large Second-Harmonic Generation and a High Laser-Induced Damage Threshold. Chemistry of Materials, 2021, 33, 6514-6521.	3.2	74
77	Linear and Nonlinear Optical Properties of $\text{K}_3\text{B}_6\text{O}_{10}\text{Br}$ Single Crystal: Experiment and Calculation. Journal of Physical Chemistry C, 2014, 118, 11849-11856.	1.5	73
78	A Series of Rare-Earth Borates $\text{K}_7\text{MRE}_2\text{B}_{15}\text{O}_{30}$ ($\text{M} = \text{Tj, ET, Q, O, Rg}$). Materials, 2018, 30, 2414-2423.	3.2	73
79	BaCdSnS_4 and $\text{Ba}_3\text{CdSn}_2\text{S}_8$: syntheses, structures, and non-linear optical and photoluminescence properties. Dalton Transactions, 2016, 45, 10681-10688.	1.6	72
80	Functional Materials Design via Structural Regulation Originated from Ions Introduction: A Study Case in Cesium Iodate System. Chemistry of Materials, 2018, 30, 1136-1145.	3.2	72
81	$\text{Na}_3\text{Cd}_3\text{B}(\text{PO}_4)_4$: A New Noncentrosymmetric Borophosphate with Zero-Dimensional Anion Units. Inorganic Chemistry, 2012, 51, 10870-10875.	1.9	71
82	The first lead fluorooxoborate $\text{PbB}_5\text{O}_8\text{F}$: achieving the coexistence of large birefringence and deep-ultraviolet cut-off edge. Chemical Communications, 2018, 54, 6308-6311.	2.2	70
83	Deep-UV Birefringent Crystal Functionalized by $[\text{B}_{12}\text{O}_{16}\text{F}_4(\text{OH})_4]$ Clusters. Angewandte Chemie - International Edition, 2022, 61, .	7.2	70
84	$\text{Pb}_7\text{O}(\text{OH})_3(\text{CO}_3)_3(\text{BO}_3)_3$: First Mixed Borate and Carbonate Nonlinear Optical Material Exhibiting Large Second-Harmonic Generation Response. Inorganic Chemistry, 2015, 54, 4138-4142.	1.9	69
85	$\text{Na}_2\text{CdGe}_2\text{Q}_6$ ($\text{Q} = \text{S, Se}$): two metal-mixed chalcogenides with phase-matching abilities and large second-harmonic generation responses. Dalton Transactions, 2017, 46, 2778-2784.	1.6	69
86	Enhancement of Birefringence in Borophosphate Pushing Phase-Matching into the Short-Wavelength Region. Journal of the American Chemical Society, 2022, 144, 9083-9090.	6.6	69
87	$(\text{NH}_4)_3\text{B}_{11}\text{PO}_{19}\text{F}_3$: a deep-UV nonlinear optical crystal with unique $[\text{B}_{10}\text{F}]^{2-}$ layers. National Science Review, 2022, 9, .	4.6	68
88	First Principle Assisted Prediction of the Birefringence Values of Functional Inorganic Borate Materials. Journal of Physical Chemistry C, 2014, 118, 25651-25657.	1.5	67
89	An investigation of new infrared nonlinear optical material: BaCdSnSe_4 , and three new related centrosymmetric compounds: Ba_2SnSe_4 , Mg_2GeSe_4 , and $\text{Ba}_2\text{Ge}_2\text{S}_6$. Dalton Transactions, 2015, 44, 19856-19864.	1.6	67
90	BaB_2S_4 : An Efficient and Air-Stable Thioborate as Infrared Nonlinear Optical Material with High Laser Damage Threshold. Chemistry of Materials, 2018, 30, 7428-7432.	3.2	67

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91	A review on phase transition and structure-performance relationship of second-order nonlinear optical polymorphs. <i>Coordination Chemistry Reviews</i> , 2020, 418, 213380.	9.5	67
92	Guanidinium Fluorooxoborates as Efficient Metal-free Short-Wavelength Nonlinear Optical Crystals. <i>Chemistry of Materials</i> , 2022, 34, 440-450.	3.2	67
93	Polar Fluorooxoborate, NaB ₄ O ₆ F: A Promising Material for Ionic Conduction and Nonlinear Optics. <i>Angewandte Chemie</i> , 2018, 130, 6687-6691.	1.6	66
94	Ba ₂ Si ₃ P ₆ : 1D Nonlinear Optical Material with Thermal Barrier Chains. <i>Journal of the American Chemical Society</i> , 2019, 141, 11976-11983.	6.6	66
95	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO ₃ /BO ₃ F Ratio in Layers. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11726-11730.	7.2	66
96	A New Lithium Rubidium Borate Li ₆ Rb ₅ B ₁₁ O ₂₂ with Isolated B ₁₁ O ₂₂ Building Blocks. <i>Crystal Growth and Design</i> , 2011, 11, 3912-3916.	1.4	64
97	A ₂ SrM ^{IV} S ₄ (A = Li, Na; M ^{IV} = Ge, Sn) concurrently exhibiting wide bandgaps and good nonlinear optical responses as new potential infrared nonlinear optical materials. <i>Chemical Science</i> , 2019, 10, 3963-3968.	3.7	64
98	NH ₄ Be ₂ BO ₃ F ₂ and β -Be ₂ BO ₃ F: Overcoming the Layering Habit in KBe ₂ BO ₃ F ₂ for the Next-Generation Deep-Ultraviolet Nonlinear Optical Materials. <i>Angewandte Chemie</i> , 2018, 130, 9106-9110.	1.6	63
99	Three new phosphates with isolated P ₂ O ₇ units: noncentrosymmetric Cs ₂ Ba ₃ (P ₂ O ₇) ₂ and centrosymmetric Cs ₂ BaP ₂ O ₇ and LiCsBaP ₂ O ₇ . <i>Dalton Transactions</i> , 2016, 45, 3936-3942.	1.6	62
100	Experimental and theoretical studies on the linear and nonlinear optical properties of lead phosphate crystals LiPbPO ₄ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19123-19129.	1.3	61
101	Two Polar Molybdenum(VI) Iodates(V) with Large Second-Harmonic Generation Responses. <i>Chemistry of Materials</i> , 2019, 31, 2992-3000.	3.2	60
102	First-Principles High-Throughput Screening Pipeline for Nonlinear Optical Materials: Application to Borates. <i>Chemistry of Materials</i> , 2020, 32, 6772-6779.	3.2	59
103	A review on the recently developed promising infrared nonlinear optical materials. <i>Dalton Transactions</i> , 2021, 50, 3155-3160.	1.6	59
104	Toward the Rational Design of Mid-Infrared Nonlinear Optical Materials with Targeted Properties via a Multi-Level Data-Driven Approach. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	58
105	Oxyhalides: prospecting ore for optical functional materials with large laser damage thresholds. <i>Journal of Materials Chemistry C</i> , 2018, 6, 2435-2442.	2.7	56
106	Nontoxic KBBF Family Member Zn ₂ BO ₃ (OH): Balance between Beneficial Layered Structure and Layer Tendency. <i>Advanced Science</i> , 2019, 6, 1901679.	5.6	56
107	Synthesis, crystal structures and optical properties of two congruent-melting isotopic diphosphates: LiM ₃ P ₂ O ₇ (M=Na, K). <i>Journal of Solid State Chemistry</i> , 2013, 197, 128-133.	1.4	55
108	Pb ₃ B ₆ O ₁₁ F ₂ : the first non-centrosymmetric lead borate fluoride with a large second harmonic generation response. <i>Journal of Materials Chemistry C</i> , 2014, 2, 1704.	2.7	55

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109	A Nitrate Nonlinear Optical Crystal $\text{Pb}_{16}(\text{OH})_{16}(\text{NO}_3)_3$ with a Large Second-Harmonic Generation Response. <i>Inorganic Chemistry</i> , 2014, 53, 3320-3325.	1.9	55
110	Contribution of lone-pairs to birefringence affected by the $\text{Pb}(\text{II})$ coordination environment: a DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21968-21973.	1.3	55
111	Experimental and Theoretical Studies on the Linear and Nonlinear Optical Properties of Bi_2ZnO_6 . <i>Journal of Physical Chemistry C</i> , 2013, 117, 14149-14157.	1.5	54
112	$\text{Na}_4\text{MgM}_2\text{Se}_6$ (M = Si, Ge): The First Noncentrosymmetric Compounds with Special Ethane-like $[\text{M}_2\text{Se}_6]^{6-}$ Units Exhibiting Large Laser-Damage Thresholds. <i>Inorganic Chemistry</i> , 2015, 54, 10108-10110.	1.9	54
113	Growth, thermal and optical properties of a novel nonlinear optical material $\text{K}_3\text{B}_6\text{O}_{10}\text{Cl}$. <i>CrystEngComm</i> , 2012, 14, 799-803.	1.3	53
114	$\text{Sr}_4\text{B}_{10}\text{O}_{18}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$: a new UV nonlinear optical material with a $[\text{B}_{10}\text{O}_{23}]^{16-}$ building block. <i>Journal of Materials Chemistry C</i> , 2014, 2, 667-674.	2.7	52
115	$p\pi$ interaction mechanism revealing and accordingly designed new member in deep-ultraviolet NLO borates $\text{Li}_n\text{M}^{n-1}\text{B}_{2n-1}\text{O}_{4n-2}$ (M = Cs/Rb, n = 3, 4). <i>J. Phys. Chem. C</i> , 2017, 121, 17843-17851.	1.9	51
116	Li_2HgMS_4 (M = Si, Ge, Sn): New Quaternary Diamond-Like Semiconductors for Infrared Laser Frequency Conversion. <i>Crystals</i> , 2017, 7, 107.	1.0	51
117	Borate Fluoride and Fluoroborate in Alkali-Metal Borate Prepared by an Open High-Temperature Solution Method. <i>Inorganic Chemistry</i> , 2014, 53, 12686-12688.	1.9	50
118	Effect of Element Substitution on Structural Transformation and Optical Performances in $\text{Li}_2\text{BaM}^{\text{IV}}\text{Q}_4$ (Li, Na, Cu, and Ag; $\text{M}^{\text{IV}} = \text{Ti, Zr, Hf, Sn, Pb, U}$). <i>J. Phys. Chem. C</i> , 2017, 121, 17843-17851.	1.9	50
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