Shilie Pan

List of Publications by Citations

465 papers	16,022 citations	59 h-index	108 g-index
511 ext. papers	20,234 ext. citations	6.2 avg, IF	7.47 L-index

#	Paper	IF	Citations
465	Finding the Next Deep-Ultraviolet Nonlinear Optical Material: NHBOF. *Journal of the American Chemical Society*, **2017**, 139, 10645-10648	16.4	601
464	K3B6O10Cl: a new structure analogous to perovskite with a large second harmonic generation response and deep UV absorption edge. *Journal of the American Chemical Society*, **2011**, 133, 7786-90	16.4	540
463	Designing a deep-ultraviolet nonlinear optical material with a large second harmonic generation response. *Journal of the American Chemical Society*, **2013**, 135, 4215-8	16.4	466
462	Fluorooxoborates: Beryllium-Free Deep-Ultraviolet Nonlinear Optical Materials without Layered Growth. *Angewandte Chemie - International Edition*, **2017**, 56, 3916-3919	16.4	451
461	CsB O F: A Congruent-Melting Deep-Ultraviolet Nonlinear Optical Material by Combining Superior Functional Units. *Angewandte Chemie - International Edition*, **2017**, 56, 14119-14123	16.4	430
460	SrB O F Functionalized with [B O F] Chromophores: Accelerating the Rational Design of Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie - International Edition*, **2018**, 57, 6095-6099	16.4	389
459	Cation-Tuned Synthesis of Fluorooxoborates: Towards Optimal Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie - International Edition*, **2018**, 57, 2150-2154	16.4	336
458	Cs3Zn6B9O21: a chemically benign member of the KBBF family exhibiting the largest second harmonic generation response. *Journal of the American Chemical Society*, **2014**, 136, 1264-7	16.4	273
457	Polar Fluorooxoborate, NaB O F: A Promising Material for Ionic Conduction and Nonlinear Optics. *Angewandte Chemie - International Edition*, **2018**, 57, 6577-6581	16.4	241
456	Recent development of metal borate halides: Crystal chemistry and application in second-order NLO materials. *Coordination Chemistry Reviews*, **2016**, 323, 15-35	23.2	231
455	A New Deep-Ultraviolet Transparent Orthophosphate LiCs2PO4 with Large Second Harmonic Generation Response. *Journal of the American Chemical Society*, **2016**, 138, 9101-4	16.4	230
454	Pb2Ba3(BO3)3Cl: A Material with Large SHG Enhancement Activated by Pb-Chelated BO3 Groups. *Journal of the American Chemical Society*, **2015**, 137, 9417-22	16.4	220
453	Designing an Excellent Deep-Ultraviolet Birefringent Material for Light Polarization. *Journal of the American Chemical Society*, **2018**, 140, 16311-16319	16.4	216
452	Cs2B4SiO9: a deep-ultraviolet nonlinear optical crystal. *Angewandte Chemie - International Edition*, **2013**, 52, 3406-10	16.4	213
451	Synthesis, crystal structure, and nonlinear optical properties of Li6CuB4O10: a congruently melting compound with isolated [CuB4O10]6- units. *Journal of the American Chemical Society*, **2006**, 128, 11631-4	16.4	211
450	Na2ZnGe2S6: A New Infrared Nonlinear Optical Material with Good Balance between Large Second-Harmonic Generation Response and High Laser Damage Threshold. *Journal of the American Chemical Society*, **2016**, 138, 7422-8	16.4	205
449	Targeting the Next Generation of Deep-Ultraviolet Nonlinear Optical Materials: Expanding from Borates to Borate Fluorides to Fluorooxoborates. *Accounts of Chemical Research*, **2019**, 52, 791-801	24.3	198

448	Borates: A Rich Source for Optical Materials. *Chemical Reviews*, **2021**, 121, 1130-1202	68.1	190
447	A novel deep UV nonlinear optical crystal Ba3B6O11F2, with a new fundamental building block, B6O14 group. *Journal of Materials Chemistry*, **2012**, 22, 9665		160
446	BaMg(BO)F polymorphs with reversible phase transition and high performances as ultraviolet nonlinear optical materials. *Nature Communications*, **2018**, 9, 3089	17.4	157
445	New Compressed Chalcopyrite-like LiBaMQ (M = Ge, Sn; Q = S, Se): Promising Infrared Nonlinear Optical Materials. *Journal of the American Chemical Society*, **2017**, 139, 14885-14888	16.4	151
444	Pb17O8Cl18: A Promising IR Nonlinear Optical Material with Large Laser Damage Threshold Synthesized in an Open System. *Journal of the American Chemical Society*, **2015**, 137, 8360-3	16.4	145
443	Na2 BaMQ4 (M=Ge, Sn; Q=S, Se): Infrared Nonlinear Optical Materials with Excellent Performances and that Undergo Structural Transformations. *Angewandte Chemie - International Edition*, **2016**, 55, 6713-5	16.4	144
442	Growth, Structure, and Properties of Single Crystals of SrBPO5. *Chemistry of Materials*, **2003**, 15, 2218-2221	9.6	143
441	Chemical Cosubstitution-Oriented Design of Rare-Earth Borates as Potential Ultraviolet Nonlinear Optical Materials. *Journal of the American Chemical Society*, **2017**, 139, 18397-18405	16.4	139
440	CsB4O6F: A Congruent-Melting Deep-Ultraviolet Nonlinear Optical Material by Combining Superior Functional Units. *Angewandte Chemie*, **2017**, 129, 14307-14311	3.6	132
439	NH Be BO F and □Be BO F: Overcoming the Layering Habit in KBe BO F for the Next-Generation Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie - International Edition*, **2018**, 57, 8968-8972	16.4	127
438	Expanding Frontiers of Ultraviolet Nonlinear Optical Materials with Fluorophosphates. *Chemistry of Materials*, **2018**, 30, 5397-5403	9.6	113
437	Emergent Deep-Ultraviolet Nonlinear Optical Candidates. *Angewandte Chemie - International Edition*, **2020**, 59, 20302-20317	16.4	104
436	Simulated pressure-induced blue-shift of phase-matching region and nonlinear optical mechanism for K3B6O10X (X = Cl, Br). *Applied Physics Letters*, **2015**, 106, 031906	3.4	101
435	Growth, Structure, and Optical Properties of a Congruent Melting Oxyborate, Bi2ZnOB2O6. *Chemistry of Materials*, **2009**, 21, 2846-2850	9.6	100
434	A new congruent-melting oxyborate, Pb4O(BO3)2 with optimally aligned BO3 triangles adopting layered-type arrangement. *Journal of Materials Chemistry*, **2012**, 22, 2105-2110		99
433	Enhancing optical anisotropy of crystals by optimizing bonding electron distribution in anionic groups. *Chemical Communications*, **2017**, 53, 2818-2821	5.8	97
432	Bi3OF3(IO3)4: Metal Oxyiodate Fluoride Featuring a Carbon-Nanotube-like Topological Structure with Large Second Harmonic Generation Response. *Chemistry of Materials*, **2017**, 29, 945-949	9.6	95
431	A Novel Nonlinear Optical Crystal Bi2ZnOB2O6. *Crystal Growth and Design*, **2009**, 9, 4091-4095	3.5	95

430	Rational Design via Synergistic Combination Leads to an Outstanding Deep-Ultraviolet Birefringent LiNaBO Material with an Unvalued BO Functional Gene. *Journal of the American Chemical Society*, **2019**, 141, 3258-3264	16.4	95
429	A congruently melting and deep UV nonlinear optical material: Li3Cs2B5O10. *Journal of Materials Chemistry*, **2011**, 21, 2890		92
428	Sn B O Cl: A Material with Large Birefringence Enhancement Activated Prepared via Alkaline-Earth-Metal Substitution by Tin. *Angewandte Chemie - International Edition*, **2019**, 58, 17675-17678	16.4	90
427	A Bulk Boron-Based Photocatalyst for Efficient Dechlorination: K3B6O10Br. *Chemistry of Materials*, **2014**, 26, 3169-3174	9.6	86
426	CaBOF: A Beryllium-Free Alkaline-Earth Fluorooxoborate Exhibiting Excellent Nonlinear Optical Performances. *Inorganic Chemistry*, **2018**, 57, 4820-4823	5.1	84
425	Cation-Tuned Synthesis of Fluorooxoborates: Towards Optimal Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie*, **2018**, 130, 2172-2176	3.6	82
424	SrB5O7F3 Functionalized with [B5O9F3]6− Chromophores: Accelerating the Rational Design of Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie*, **2018**, 130, 6203-6207	3.6	80
423	The first quaternary diamond-like semiconductor with 10-membered LiS rings exhibiting excellent nonlinear optical performances. *Chemical Communications*, **2017**, 53, 3010-3013	5.8	79
422	UV nonlinear optical crystal Ba2[B6O9(OH)4] featuring unique chiral layers with a new B18O42 circle based on BO3 and BO4 units. *Inorganic Chemistry*, **2012**, 51, 1852-8	5.1	77
421	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. *Journal of the American Chemical Society*, **2018**, 140, 10726-10733	16.4	76
420	Crystal growth and optical properties of a noncentrosymmetric haloid borate, K3B6O10Br. *CrystEngComm*, **2011**, 13, 2899	3.3	76
419	Fluorooxoborates: Beryllium-Free Deep-Ultraviolet Nonlinear Optical Materials without Layered Growth. *Angewandte Chemie*, **2017**, 129, 3974-3977	3.6	74
418	Li4Cs3B7O14: synthesis, crystal structure, and optical properties. *Inorganic Chemistry*, **2011**, 50, 2415-9	5.1	74
417	Synthesis, structure, and properties of the noncentrosymmetric hydrated borate Na(2)B(5)O(8)(OH).2H(2)O. *Inorganic Chemistry*, **2009**, 48, 7800-4	5.1	72
416	KPb2(PO3)5: a novel nonlinear optical lead polyphosphate with a short deep-UV cutoff edge. *Journal of Materials Chemistry C*, **2016**, 4, 10630-10637	7.1	71
415	NaBOF: A Fluoroborate with Short Cutoff Edge and Deep-Ultraviolet Birefringent Property Prepared by an Open High-Temperature Solution Method. *Inorganic Chemistry*, **2017**, 56, 344-350	5.1	70
414	Na3Cd3B(PO4)4: a new noncentrosymmetric borophosphate with zero-dimensional anion units. *Inorganic Chemistry*, **2012**, 51, 10870-5	5.1	68
413	Polar Polymorphism: □ □ and □Pb2Ba4Zn4B14O31□Synthesis, Characterization, and Nonlinear Optical Properties. *Chemistry of Materials*, **2015**, 27, 4779-4788	9.6	67

412	Module-Analysis-Assisted Design of Deep Ultraviolet Fluorooxoborates with Extremely Large Gap and High Structural Stability. *Chemistry of Materials*, **2019**, 31, 2807-2813	9.6	66
411	Cs4Mo5P2O22: a first Strandberg-type POM with 1D straight chains of polymerized [Mo5P2O23]6- units and moderate second harmonic generation response. *Chemical Communications*, **2013**, 49, 306-8	5.8	65
410	Linear and Nonlinear Optical Properties of K3B6O10Br Single Crystal: Experiment and Calculation. *Journal of Physical Chemistry C*, **2014**, 118, 11849-11856	3.8	62
409	A New Lithium Rubidium Borate Li6Rb5B11O22with Isolated B11O22Building Blocks. *Crystal Growth and Design*, **2011**, 11, 3912-3916	3.5	62
408	Deep-Ultraviolet Nonlinear-Optical Material KSrLiAlBOF: Addressing the Structural Instability Problem in KBeBOF. *Inorganic Chemistry*, **2017**, 56, 8755-8758	5.1	61
407	Fluorooxoborates: Ushering in a New Era of Deep Ultraviolet Nonlinear Optical Materials. *Chemistry - A European Journal*, **2018**, 24, 17638-17650	4.8	60
406	LiRb2PO4: a new deep-ultraviolet nonlinear optical phosphate with a large SHG response. *Journal of Materials Chemistry C*, **2017**, 5, 269-274	7.1	59
405	First Principle Assisted Prediction of the Birefringence Values of Functional Inorganic Borate Materials. *Journal of Physical Chemistry C*, **2014**, 118, 25651-25657	3.8	59
404	NaCdGeQ (Q = S, Se): two metal-mixed chalcogenides with phase-matching abilities and large second-harmonic generation responses. *Dalton Transactions*, **2017**, 46, 2778-2784	4.3	57
403	Pb7O(OH)3(CO3)3(BO3): first mixed borate and carbonate nonlinear optical material exhibiting large second-harmonic generation response. *Inorganic Chemistry*, **2015**, 54, 4138-42	5.1	57
402	Three new phosphates with isolated P2O7 units: noncentrosymmetric Cs2Ba3(P2O7)2 and centrosymmetric Cs2BaP2O7 and LiCsBaP2O7. *Dalton Transactions*, **2016**, 45, 3936-42	4.3	57
401	BaCdSnS4 and Ba3CdSn2S8: syntheses, structures, and non-linear optical and photoluminescence properties. *Dalton Transactions*, **2016**, 45, 10681-8	4.3	56
400	The first lead fluorooxoborate PbBOF: achieving the coexistence of large birefringence and deep-ultraviolet cut-off edge. *Chemical Communications*, **2018**, 54, 6308-6311	5.8	55
399	Polar Fluorooxoborate, NaB4O6F: A Promising Material for Ionic Conduction and Nonlinear Optics. *Angewandte Chemie*, **2018**, 130, 6687-6691	3.6	54
398	Advantageous Units in Antimony Sulfides: Exploration and Design of Infrared Nonlinear Optical Materials. *ACS Applied Materials & Interfaces*, **2018**, 10, 26413-26421	9.5	54
397	A Series of Rare-Earth Borates K7MRE2B15O30 (M = Zn, Cd, Pb; RE = Sc, Y, Gd, Lu) with Large Second Harmonic Generation Responses. *Chemistry of Materials*, **2018**, 30, 2414-2423	9.6	53
396	ASrMS (A = Li, Na; M = Ge, Sn) concurrently exhibiting wide bandgaps and good nonlinear optical responses as new potential infrared nonlinear optical materials. *Chemical Science*, **2019**, 10, 3963-3968	9.4	52
395	Experimental and Theoretical Studies on the Linear and Nonlinear Optical Properties of Bi2ZnOB2O6. *Journal of Physical Chemistry C*, **2013**, 117, 14149-14157	3.8	52

394	CsAlBOF: a beryllium-free deep-ultraviolet nonlinear optical material with enhanced thermal stability. *Chemical Science*, **2019**, 11, 694-698	9.4	52
393	Functional Materials Design via Structural Regulation Originated from Ions Introduction: A Study Case in Cesium Iodate System. *Chemistry of Materials*, **2018**, 30, 1136-1145	9.6	51
392	An investigation of new infrared nonlinear optical material: BaCdSnSe4, and three new related centrosymmetric compounds: Ba2SnSe4, Mg2GeSe4, and Ba2Ge2S6. *Dalton Transactions*, **2015**, 44, 19856-64	4.3	50
391	Experimental and theoretical studies on the linear and nonlinear optical properties of lead phosphate crystals LiPbPO4. *Physical Chemistry Chemical Physics*, **2016**, 18, 19123-9	3.6	50
390	Growth, thermal and optical properties of a novel nonlinear optical material K3B6O10Cl. *CrystEngComm*, **2012**, 14, 799-803	3.3	49
389	Pb3B6O11F2: the first non-centrosymmetric lead borate fluoride with a large second harmonic generation response. *Journal of Materials Chemistry C*, **2014**, 2, 1704	7.1	48
388	A nitrate nonlinear optical crystal Pb16(OH)16(NO3)16 with a large second-harmonic generation response. *Inorganic Chemistry*, **2014**, 53, 3320-5	5.1	48
387	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO /BO F Ratio in Layers. *Angewandte Chemie - International Edition*, **2019**, 58, 11726-11730	16.4	47
386	Synthesis, crystal structures and optical properties of two congruent-melting isotypic diphosphates: LiM3P2O7 (M=Na, K). *Journal of Solid State Chemistry*, **2013**, 197, 128-133	3.3	47
385	p□(b,□) interaction mechanism revealing and accordingly designed new member in deep-ultraviolet NLO borates LinMn□B2n□O4n□ (M = Cs/Rb, n = 3, 4, 6). *Journal of Materials Chemistry C*, **2014**, 2, 4133-4141	7.1	46
384	Ba4(BO3)3(SiO4)□Ba3X (X = Cl, Br): new salt-inclusion borosilicate halides as potential deep UV nonlinear optical materials. *Journal of Materials Chemistry C*, **2014**, 2, 4257	7.1	45
383	BaB2S4: An Efficient and Air-Stable Thioborate as Infrared Nonlinear Optical Material with High Laser Damage Threshold. *Chemistry of Materials*, **2018**, 30, 7428-7432	9.6	45
382	Na4MgM2Se6 (M = Si, Ge): The First Noncentrosymmetric Compounds with Special Ethane-like [M2Se6](6-) Units Exhibiting Large Laser-Damage Thresholds. *Inorganic Chemistry*, **2015**, 54, 10108-10	5.1	44
381	PbB5O7F3: A High-Performing Short-Wavelength Nonlinear Optical Material. *Chemistry of Materials* , **2020**, 32, 2172-2179	9.6	44
380	Further examples of the P-O-P connection in borophosphates: synthesis and characterization of Li2Cs2B2P4O15, LiK2BP2O8, and Li3M2BP4O14 (M = K, Rb). *Chemistry - A European Journal*, **2012**, 18, 12046-51	4.8	43
379	Two Polar Molybdenum(VI) Iodates(V) with Large Second-Harmonic Generation Responses. *Chemistry of Materials*, **2019**, 31, 2992-3000	9.6	42
378	Noncentrosymmetric versus Centrosymmetric: Influence of the Na+ Substitution on Structural Transition and Second-Harmonic Generation Property. *Crystal Growth and Design*, **2014**, 14, 1794-1801	3.5	42
377	Sr4B10O18(OH)2□2H2O: a new UV nonlinear optical material with a [B10O23]16□building block. *Journal of Materials Chemistry C*, **2014**, 2, 667-674	7.1	42

376	NH4Be2BO3F2 and □Be2BO3F: Overcoming the Layering Habit in KBe2BO3F2 for the Next-Generation Deep-Ultraviolet Nonlinear Optical Materials. *Angewandte Chemie*, **2018**, 130, 9106-9110	3.6	42
375	Synthesis and characterization of mid-infrared transparency compounds: acentric BaHgS2 and centric Ba8Hg4S5Se7. *Inorganic Chemistry*, **2015**, 54, 2772-9	5.1	41
374	Enhanced nonlinear optical functionality in birefringence and refractive index dispersion of the deep-ultraviolet fluorooxoborates. *Science China Materials*, **2020**, 63, 1480-1488	7.1	41
373	Na2BaMQ4 (M=Ge, Sn; Q=S, Se): Infrared Nonlinear Optical Materials with Excellent Performances and that Undergo Structural Transformations. *Angewandte Chemie*, **2016**, 128, 6825-6827	3.6	41
372	Ba2B10O17: a new centrosymmetric alkaline-earth metal borate with a deep-UV cut-off edge. *Dalton Transactions*, **2014**, 43, 8905-10	4.3	41
371	BaB8O12F2: a promising deep-UV birefringent material. *Inorganic Chemistry Frontiers*, **2019**, 6, 546-549	6.8	40
370	A review on phase transition and structure-performance relationship of second-order nonlinear optical polymorphs. *Coordination Chemistry Reviews*, **2020**, 418, 213380	23.2	40
369	BaSiP: 1D Nonlinear Optical Material with Thermal Barrier Chains. *Journal of the American Chemical Society*, **2019**, 141, 11976-11983	16.4	40
368	Borate fluoride and fluoroborate in alkali-metal borate prepared by an open high-temperature solution method. *Inorganic Chemistry*, **2014**, 53, 12686-8	5.1	40
367	New salt-inclusion borate, Li3Ca9(BO3)7□2[LiF]: a promising UV NLO material with the coplanar and high density BO3 triangles. *Inorganic Chemistry*, **2013**, 52, 5359-65	5.1	40
366	Effect of Element Substitution on Structural Transformation and Optical Performances in IBaMQ (I = Li, Na, Cu, and Ag; M = Si, Ge, and Sn; Q = S and Se). *Inorganic Chemistry*, **2018**, 57, 3434-3442	5.1	39
365	Oxyhalides: prospecting ore for optical functional materials with large laser damage thresholds. *Journal of Materials Chemistry C*, **2018**, 6, 2435-2442	7.1	39
364	Flux growth and characterization of a new oxyborate crystal Na3La9O3(BO3)8. *Journal of Crystal Growth*, **2005**, 275, e1997-e2001	1.6	39
363	Contribution of lone-pairs to birefringence affected by the Pb(II) coordination environment: a DFT investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 21968-73	3.6	38
362	BaCu2MIVQ4 (MIV = Si, Ge, and Sn; Q = S, Se): synthesis, crystal structures, optical performances and theoretical calculations. *RSC Advances*, **2017**, 7, 29378-29385	3.7	37
361	Effect of Rigid Units on the Symmetry of the Framework: Design and Synthesis of Centrosymmetric NaBa4(B5O9)2F2Cl and Noncentrosymmetric NaBa4(AlB4O9)2Br3. *Crystal Growth and Design*, **2013** , 13, 3514-3521	3.5	37
360	Cs2B4SiO9: A Deep-Ultraviolet Nonlinear Optical Crystal. *Angewandte Chemie*, **2013**, 125, 3490-3494	3.6	37
359	BaClBF4: a new noncentrosymmetric pseudo-Aurivillius type material with transparency range from deep UV to middle IR and a high laser damage threshold. *Journal of Materials Chemistry C*, **2013**, 1, 4740	7.1	35

358	Structure-property survey and computer-assisted screening of mid-infrared nonlinear optical chalcohalides. *Coordination Chemistry Reviews*, **2020**, 421, 213379	23.2	35
357	Q18Mg6(B5O10)3(B7O14)2F (Q = Rb and Cs): new borates containing two large isolated polyborate anions with similar topological structures. *Chemistry - A European Journal*, **2015**, 21, 1414-9	4.8	34
356	Li2HgMS4 (M = Si, Ge, Sn): New Quaternary Diamond-Like Semiconductors for Infrared Laser Frequency Conversion. *Crystals*, **2017**, 7, 107	2.3	33
355	Synthesis, crystal growth and characterization of a new noncentrosymmetric borophosphate: RbPbBP2O8. *CrystEngComm*, **2013**, 15, 4956	3.3	33
354	Synthesis, crystal structure, and nonlinear optical properties of Bi2Cu5B4O14. *Journal of Solid State Chemistry*, **2008**, 181, 2087-2091	3.3	33
353	Toward the Enhancement of Critical Performance for Deep-Ultraviolet Frequency-Doubling Crystals Utilizing Covalent Tetrahedra. *Accounts of Materials Research*, **2021**, 2, 282-291	7.5	33
352	Nontoxic KBBF Family Member ZnBO(OH): Balance between Beneficial Layered Structure and Layer Tendency. *Advanced Science*, **2019**, 6, 1901679	13.6	32
351	Ce(IO) F ?H O: The First Rare-Earth-Metal Iodate Fluoride with Large Second Harmonic Generation Response. *Chemistry - A European Journal*, **2019**, 25, 1221-1226	4.8	32
350	The lone-pairs enhanced birefringence and SHG response: A DFT investigation on M2B5O9Cl (M=Sr, Ba, and Pb). *Chemical Physics*, **2015**, 453-454, 42-46	2.3	31
349	Designing excellent mid-infrared nonlinear optical materials with fluorooxo-functional group of d0 transition metal oxyfluorides. *Science China Materials*, **2019**, 62, 1798-1806	7.1	31
348	Synthesis, crystal structure and optical properties of the new lead fluoride borate Pb2BO3F. *Journal of Solid State Chemistry*, **2011**, 184, 2849-2853	3.3	31
347	SnF : A UV Birefringent Material with Large Birefringence and Easy Crystal Growth. *Angewandte Chemie - International Edition*, **2021**, 60, 3540-3544	16.4	31
346	Designing Deep-UV Birefringent Crystals by Cation Regulation. *Chemistry - A European Journal*, **2018**, 24, 11267-11272	4.8	31
345	Synthesis and Structure of KPbBP2O8 A Congruent Melting Borophosphate with Nonlinear Optical Properties. *European Journal of Inorganic Chemistry*, **2013**, 2013, 3185-3190	2.3	30
344	Discovery of First Magnesium Fluorooxoborate with Stable Fluorine Terminated Framework for Deep-UV Nonlinear Optical Application. *Angewandte Chemie - International Edition*, **2021**, 60, 14650-14656	16.4	30
343	Li MgGe S : The First Alkali and Alkaline-Earth Diamond-Like Infrared Nonlinear Optical Material with Exceptional Large Band Gap. *Angewandte Chemie - International Edition*, **2021**, 60, 24131-24136	16.4	30
342	New molybdenum(VI) phosphates: synthesis, characterization, and calculations of centrosymmetric RbMoO2PO4 and noncentrosymmetric Rb4Mo5P2O22. *Inorganic Chemistry*, **2013**, 52, 1488-95	5.1	29
341	First-Principles High-Throughput Screening Pipeline for Nonlinear Optical Materials: Application to Borates. *Chemistry of Materials*, **2020**, 32, 6772-6779	9.6	29

340	Mg?Si?As: An Unexplored System with Promising Nonlinear Optical Properties. *Advanced Functional Materials*, **2018**, 28, 1801589	15.6	29
339	K B O F : A New Fluorooxoborate with Four Different Anionic Units. *Chemistry - A European Journal*, **2018**, 24, 4497-4502	4.8	28
338	Synthesis, Characterization, and Theoretical Studies of (Pb4O)Pb2B6O14: A New Lead(II) Borate with Isolated Oxygen-Centered Pb4O Tetrahedra and Large Second Harmonic Generation Response. *Journal of Physical Chemistry C*, **2016**, 120, 12757-12764	3.8	28
337	Li3AlSiO5: the first aluminosilicate as a potential deep-ultraviolet nonlinear optical crystal with the quaternary diamond-like structure. *Physical Chemistry Chemical Physics*, **2016**, 18, 4362-9	3.6	28
336	Pb2B5O9Cl: a chloride borate with second harmonic generation effect. *Journal of Materials Science*, **2013**, 48, 2590-2596	4.3	28
335	Expanding the chemistry of borates with functional [BO] anions. *Nature Communications*, **2021**, 12, 2597	17.4	28
334	ASrPO (A = Rb, Cs): Two Polyphosphates Based on Different Types of P-O Chains and Ring Structures. *Inorganic Chemistry*, **2017**, 56, 3939-3945	5.1	27
333	Infrared Nonlinear Optical Polymorphs □and □SrCu2SnS4 Exhibiting Large Second Harmonic Generation Responses with Requisite Phase-Matching Behavior. *Chemistry of Materials*, **2020**, 32, 1281-1287	9.6	27
332	Series of Crystals with Giant Optical Anisotropy: A Targeted Strategic Research. *Angewandte Chemie - International Edition*, **2021**, 60, 1332-1338	16.4	27
331	Ban+2Znn(BO3)n(B2O5)Fn (n = 1, 2): new members of the zincoborate fluoride series with two kinds of isolated B□ units. *Inorganic Chemistry Frontiers*, **2017**, 4, 281-288	6.8	26
330	LiNaCsBO: a new edge-sharing [BO] tetrahedra containing borate with high anisotropic thermal expansion. *Chemical Communications*, **2019**, 55, 1295-1298	5.8	26
329	Anomalous second-harmonic generation response in SrBPO5 and BaBPO5. *Journal of Materials Chemistry C*, **2015**, 3, 1557-1566	7.1	26
328	Nonlinear electronic polarization and optical response in borophosphate BPO4. *Physical Review B*, **2016**, 93,	3.3	26
327	New type of complex alkali and alkaline earth metal borates with isolated (B12O24)12) anionic group. *Dalton Transactions*, **2014**, 43, 4886-91	4.3	26
326	Effect of halogen (Cl, Br) on the symmetry of flexible perovskite-related framework. *Inorganic Chemistry*, **2014**, 53, 11213-20	5.1	26
325	Synthesis, structure characterization and optical properties of a new lead cadmium borate. *Inorganica Chimica Acta*, **2012**, 384, 158-162	2.7	26
324	Structure and magnetic properties of Pb2Cu3B4O11: a new copper borate featuring [Cu3O8]10- units. *Inorganic Chemistry*, **2007**, 46, 3851-5	5.1	26
323	Neue Kandidaten f□die nichtlineare Optik im Tief-UV-Bereich. *Angewandte Chemie*, **2020**, 132, 20480-20486	3.6	26

322	Top-Seeded Solution Crystal Growth and Linear and Nonlinear Optical Properties of Ba4B11O20F. *Crystal Growth and Design*, **2017**, 17, 1404-1410	3.5	25
321	M2Cd3B16O28 (M = Rb, Cs): Two Isostructural Alkali Cadmium Borates with a New Type of Borate Layer. *European Journal of Inorganic Chemistry*, **2013**, 2013, 203-207	2.3	25
320	LiZnGeS: a promising diamond-like infrared nonlinear optical material with high laser damage threshold and outstanding second-harmonic generation response. *Dalton Transactions*, **2019**, 48, 4484-4488	4.3	25
319	Hydroxyfluorooxoborate Na[B O F (OH)]?[B(OH)]: Optimizing the Optical Anisotropy with Heteroanionic Units for Deep Ultraviolet Birefringent Crystals. *Angewandte Chemie - International Edition*, **2021**, 60, 20469-20475	16.4	25
318	Three Mixed-Alkaline Borates: NaMBO (M = Rb, Cs) with Two Interpenetrating Three-Dimensional B-O Networks and LiCsBO with Fundamental Building Block BO. *Inorganic Chemistry*, **2017**, 56, 13456-13463	5.1	24
317	Ba2GeS4 and Mg2SnS4: synthesis, structures, optical properties and electronic structures. *RSC Advances*, **2015**, 5, 33646-33652	3.7	24
316	Synthesis and optical properties of the first lead borate bromide with isolated BO3 groups: Pb2Ba3(BO3)3Br. *Dalton Transactions*, **2015**, 44, 16818-23	4.3	24
315	Computer-Assisted Design of a Superior BeBOF Deep-Ultraviolet Nonlinear-Optical Material. *Inorganic Chemistry*, **2018**, 57, 5716-5719	5.1	24
314	A Fluorooxosilicophosphate with an Unprecedented SiO F Species. *Angewandte Chemie - International Edition*, **2018**, 57, 9828-9832	16.4	24
313	Pb4Zn2B10O21: a congruently melting lead zinc borate with a novel [B10O24] anionic group and an interesting [Pb4O12]□chain. *New Journal of Chemistry*, **2014**, 38, 285-291	3.6	24
312	Structural insights for the design of new borate-phosphates: synthesis, crystal structure and optical properties of Pb□(BO□)(PO□)and Bi□□(BO□)(PO□). *Dalton Transactions*, **2014**, 43, 12886-93	4.3	24
311	Fluorine-Driven Enhancement of Birefringence in the Fluorooxosulfate: A Deep Evaluation from a Joint Experimental and Computational Study. *Advanced Science*, **2021**, 8, e2003594	13.6	24
310	NaMBO (M = Rb and Cs): Noncentrosymmetric Borates with Unprecedented [BO] Fundamental Building Blocks. *Inorganic Chemistry*, **2017**, 56, 5506-5509	5.1	23
309	ABaSbQ (A = Li, Na; Q = S, Se): diverse arrangement modes of isolated SbQ ligands regulating the magnitudes of birefringences. *Chemical Communications*, **2019**, 55, 5143-5146	5.8	23
308	New Alkaline-Earth Metal Fluoroiodates Exhibiting Large Birefringence and Short Ultraviolet Cutoff Edge with Highly Polarizable (IO3F)2□Units. *Chemistry of Materials*, **2020**, 32, 5723-5728	9.6	23
307	BaBOF: a new aurivillius-like borate containing two types of F atoms. *Dalton Transactions*, **2018**, 47, 5157-5160	4.3	23
306	From LiB O to NaRbB O F : Fluorine-Directed Evolution of Structural Chemistry. *Chemistry - A European Journal*, **2018**, 24, 10022	4.8	23
305	Second-harmonic generation in noncentrosymmetric phosphates. *Physical Review B*, **2017**, 96,	3.3	23

304	Synthesis, characterization and theoretical studies of nonlinear optical crystal Sr2B5O9(OH)□H2O. *Physical Chemistry Chemical Physics*, **2015**, 17, 10489-96	3.6	23
303	Li5Rb2B7O14: a new congruently melting compound with two kinds of B□O one-dimensional chains and short UV absorption edge. *CrystEngComm*, **2012**, 14, 6720	3.3	23
302	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. *Physical Review Letters*, **2020**, 125, 187402	7.4	23
301	□CsB O : A Triple-Layered Borate with Edge-Sharing BO Tetrahedra Exhibiting a Short Cutoff Edge and a Large Birefringence. *Chemistry - A European Journal*, **2019**, 25, 11614-11619	4.8	22
300	BaB O F : A Barium Fluorooxoborate with a Unique [B O F] Layer and Short Cutoff Edge. *Chemistry - A European Journal*, **2019**, 25, 6693-6697	4.8	22
299	Effect of the cation size on the framework structures of magnesium tungstate, A4Mg(WO4)3 (A = Na, K), R2Mg2(WO4)3 (R = Rb, Cs). *Dalton Transactions*, **2015**, 44, 5810-7	4.3	22
298	Structural Insights into Borates with an Anion-Templated Open-Framework Configuration: Asymmetric K BaB O versus Centrosymmetric K CsB O and Na M NB O (M=Rb, Cs; N=Ba, Pb). *Chemistry - A European Journal*, **2017**, 23, 13910-13918	4.8	22
297	Na11B21O36X2 (X = Cl, Br): halogen sodium borates with a new graphene-like borate double layer. *Chemistry - A European Journal*, **2013**, 19, 7338-41	4.8	22
296	Effects of the Orientation of [BO] Fundamental Building Blocks on Layered Structures Based on the Pentaborates. *Inorganic Chemistry*, **2016**, 55, 10608-10616	5.1	22
295	Sn2B5O9Cl: A Material with Large Birefringence Enhancement Activated Prepared via Alkaline-Earth-Metal Substitution by Tin. *Angewandte Chemie*, **2019**, 131, 17839-17842	3.6	21
294	New tartratoborates: synthesis, structure, and characterization of non-centrosymmetric ASr[C4H2O6B(OH)2]□4H2O (A = K+, Rb+). *Journal of Materials Chemistry A*, **2013**, 1, 10389	13	21
293	Sr3B6O11F2: a promising polar fluoroborate with short UV absorption edge and moderate second harmonic generation response. *Scripta Materialia*, **2013**, 69, 449-452	5.6	21
292	MBaYBO (M = Rb, Cs): two new rare-earth borates with large birefringence and short ultraviolet cutoff edges. *Dalton Transactions*, **2018**, 47, 750-757	4.3	21
291	MMPO (M = Rb, M = Cd, Mg, Ca; M = Cs, M = Pb, Sr; M = K, M = Mg): Cation Substitution Application in Cyclophosphate Family and Nonlinear Optical Properties. *Inorganic Chemistry*, **2018**, 57, 7372-7379	5.1	21
290	Theoretical perspective of the lone pair activity influence on band gap and SHG response of lead borates. *RSC Advances*, **2015**, 5, 79882-79887	3.7	20
289	ZnIOF: Zinc Iodate Fluoride with Large Birefringence and Wide Band Gap. *Inorganic Chemistry*, **2020**, 59, 4172-4175	5.1	20
288	Predicting Global Minimum in Complex Beryllium Borate System for Deep-ultraviolet Functional Optical Applications. *Scientific Reports*, **2016**, 6, 34839	4.9	20
287	Synthesis, structures, optical properties and electronic structures of two mixed metal borates MBaB5O9 (M = Na, K). *Journal of Alloys and Compounds*, **2014**, 585, 602-607	5.7	20

286	The interaction between cations and anionic groups inducing SHG enhancement in a series of apatite-like crystals: A first-principles study. *Journal of Solid State Chemistry*, **2014**, 219, 138-142	3.3	20
285	Flux growth of BPO4 crystals. *Journal of Crystal Growth*, **2004**, 270, 486-490	1.6	20
284	A New Nonlinear Optical Borate Crystal Na3La2(BO3)3. *Chemistry Letters*, **2001**, 30, 456-457	1.7	20
283	A new family of quaternary thiosilicates SrA2SiS4 (A = Li, Na, Cu) as promising infrared nonlinear optical crystals. *Journal of Materials Chemistry C*, **2020**, 8, 1762-1767	7.1	20
282	Effect of the [Ba2BO3F]□Layer on the Band Gap: Synthesis, Characterization, and Theoretical Studies of BaZn2B2O6□hBa2BO3F (n = 0, 1, 2). *Inorganic Chemistry*, **2016**, 55, 4806-12	5.1	20
281	Strong Nonlinearity Induced by Coaxial Alignment of Polar Chain and Dense [BO3] Units in CaZn2(BO3)2.. *Angewandte Chemie - International Edition*, **2022**,	16.4	20
280	Na6Zn3MIII2Q9 (MIII = Ga, In; Q = S, Se): four new supertetrahedron-layered chalcogenides with unprecedented vertex-sharing T3-clusters and desirable photoluminescence performances. *Inorganic Chemistry Frontiers*, **2018**, 5, 1415-1422	6.8	19
279	NaBa4(GaB4O9)2X3 (X = Cl, Br) with NLO-Active GaO4 Tetrahedral Unit: Experimental and ab Initio Studies. *Journal of Physical Chemistry C*, **2016**, 120, 6190-6197	3.8	19
278	Prediction and Characterization of NaGaS, A High Thermal Conductivity Mid-Infrared Nonlinear Optical Material for High-Power Laser Frequency Conversion. *Inorganic Chemistry*, **2019**, 58, 93-98	5.1	19
277	Exploring the influence of cationic skeletons on the arrangement of isolated BO3 groups based on RbMgBO3, CsZn4(BO3)3 and Cs4Mg4(BO3)4. *New Journal of Chemistry*, **2014**, 38, 3035-3041	3.6	19
276	Li2Sr4B12O23: A new alkali and alkaline-earth metal mixed borate with [B10O18]6□network and isolated [B2O5]4□unit. *Journal of Solid State Chemistry*, **2012**, 190, 92-97	3.3	19
275	Pb6Ba2(BO3)5X (X = Cl, Br): new borate halides with strong predicted optical anisotropies derived from Pb(2+) and (BO3)(3.). *Dalton Transactions*, **2015**, 44, 7041-7	4.3	19
274	Synthesis, crystal structure and optical properties of a novel sodium lead pentaborate, NaPbB5O9. *Journal of Solid State Chemistry*, **2011**, 184, 825-829	3.3	19
273	Finding Optimal Mid-Infrared Nonlinear Optical Materials in Germanates by First-Principles High-Throughput Screening and Experimental Verification. *ACS Applied Materials & Interfaces*, **2020**, 12, 45023-45035	9.5	19
272	Design and Syntheses of Three Novel Carbonate Halides: Cs3 Pb2 (CO3)3 I, KBa2 (CO3)2 F, and RbBa2 (CO3)2 F. *Chemistry - A European Journal*, **2016**, 22, 2944-54	4.8	19
271	A review on the recently developed promising infrared nonlinear optical materials. *Dalton Transactions*, **2021**, 50, 3155-3160	4.3	19
270	Hg3P2S8: 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	9.6	19
269	Growth, Properties, and Theoretical Analysis of MLiVO (M = Rb, Cs) Crystals: Two Potential Mid-Infrared Nonlinear Optical Materials. *Scientific Reports*, **2017**, 7, 1901	4.9	18

268	The mechanism of large second harmonic generation enhancement activated by Zn substitution. *Physical Chemistry Chemical Physics*, **2016**, 18, 32931-32936	3.6	18
267	Li(0.8)Mg(2.1)B2O5F: the first borate fluoride with magnesium-oxygen-fluorine octahedral chains. *Dalton Transactions*, **2014**, 43, 2828-34	4.3	18
266	Synthesis, crystal structure and characterization of a new compound, Li3NaBaB6O12. *Solid State Sciences*, **2012**, 14, 1186-1190	3.4	18
265	Synthesis, crystal structure and optical properties of a new lead fluoride borate with isolated [B9O21]15□unit. *Inorganic Chemistry Communication*, **2011**, 14, 566-568	3.1	18
264	K3B3O4(OH)4□2H2O: A UV Nonlinear Optical Crystal with Isolated [B3O4(OH)4](3-) Anion Groups. *Inorganic Chemistry*, **2016**, 55, 8744-9	5.1	18
263	A review on the development of infrared nonlinear optical materials with triangular anionic groups. *Journal of Solid State Chemistry*, **2019**, 271, 266-272	3.3	18
262	Experimental characterization and first principles calculations of linear and nonlinear optical properties of two orthophosphates A3Al2(PO4)3 (A = Rb, K). *Inorganic Chemistry Frontiers*, **2019**, 6, 504-510	6.8	17
261	Synthesis, characterization, and theoretical analysis of three new nonlinear optical materials K7MRE2B15O30 (M= Ca and Ba, RE= La and Bi). *Science China Materials*, **2019**, 62, 1151-1161	7.1	17
260	Ba4M(CO3)2(BO3)2 (M=Ba, Sr): two borate-carbonates synthesized by open high temperature solution method. *Science China Materials*, **2019**, 62, 1023-1032	7.1	17
259	K7B2P5O19: a novel alkali metal borophosphate with zero dimensional [B2P5O19]7□anionic units. *CrystEngComm*, **2014**, 16, 6848-6851	3.3	17
258	Noncentrosymmetric Cubic CsCdBO3 with Bichromophore. *European Journal of Inorganic Chemistry*, **2013**, 2013, 5528-5533	2.3	17
257	The effect of 1-N-alkyl chain of ionic liquids [Cnmim]+Br□(n = 2, 4, 6, 8) on the aspect ratio of ZnO nanorods: syntheses, morphology, forming mechanism, photoluminescence and recyclable photocatalytic activity. *Journal of Materials Chemistry*, **2011**, 21, 15732		17
256	Crystal growth and characterization of K2B4O11H8. *Journal of Crystal Growth*, **2009**, 311, 3517-3521	1.6	17
255	A review of the ABCD family as infrared nonlinear optical materials: the effect of each site on the structure and optical properties. *Chemical Communications*, **2020**, 56, 11565-11576	5.8	17
254	Sn2B5O9Br as an Outstanding Bifunctional Material with Strong Second-Harmonic Generation Effect and Large Birefringence. *Advanced Optical Materials*, **2021**, 9, 2001734	8.1	17
253	ACaBO (A = Cs, Rb): two new cubic borates with isolated BO groups. *Dalton Transactions*, **2017**, 46, 4968-4974	4.0	16
252	Transformation of the B-O Units from Corner-Sharing to Edge-Sharing Linkages in BaMBO (M = Ga, Al). *Inorganic Chemistry*, **2019**, 58, 8237-8244	5.1	16
251	A new barium fluorooxoborate BaBOF□xHO with large birefringence and a wide UV transparency window. *Dalton Transactions*, **2019**, 48, 6714-6717	4.3	16

250	Cs6RE2(PO4)4 (RE = Y and Gd): two new members of the alkali rare-earth double phosphates. *New Journal of Chemistry*, **2015**, 39, 4328-4333	3.6	16
249	K2Na(IO3)2(I3O8) with Strong Second Harmonic Generation Response Activated by Two Types of Isolated Iodate Anions. *Chemistry of Materials*, **2020**, 32, 3608-3614	9.6	16
248	Four new quaternary chalcogenides A2Ba7Sn4Q16 (A = Li, Na; Q = S, Se): syntheses, crystal structures determination, nonlinear optical performances investigation. *New Journal of Chemistry*, **2018**, 42, 3350-3355	3.6	16
247	A Member of Fluorooxoborates: LiNaKBOF with the Fundamental Building Block BOF and a Short Cutoff Edge. *Inorganic Chemistry*, **2018**, 57, 873-878	5.1	16
246	KRbBO: a new triple-layered borate with an unprecedented [BO] fundamental building block. *Dalton Transactions*, **2018**, 47, 10833-10836	4.3	16
245	The influence of hydrogen bonding on the nonlinear optical properties of a semiorganic material NH4B[D-(+)-C4H4O5]2□H2O: a theoretical perspective. *Physical Chemistry Chemical Physics*, **2014**, 16, 20089-96	3.6	16
244	Optical properties of BaBPO_5 crystals. *Journal of the Optical Society of America B: Optical Physics*, **2004**, 21, 761	1.7	16
243	A High Laser Damage Threshold and a Good Second-Harmonic Generation Response in a New Infrared NLO Material: LiSm3SiS7. *Crystals*, **2016**, 6, 121	2.3	16
242	Application of the Dimensional Reduction Formalism to Pb12[Li2(P2O7)2(P4O13)2](P4O13): a Phosphate Containing Three Types of Isolated P-O Groups. *Inorganic Chemistry*, **2016**, 55, 7329-31	5.1	16
241	Remarkable multimember-ring configurations in a new family of NaMSbS (M = Zn, Cd, Hg) exhibiting various three-dimensional tunnel structures. *Chemical Communications*, **2018**, 54, 8269-8272	5.8	16
240	Effect of cation substitution on structural transition: synthesis, characterization and theoretical studies of NaCa4B3O9, NaCaBO3, NaSrBO3 and Li4CaB2O6. *Physical Chemistry Chemical Physics*, **2015**, 17, 26359-68	3.6	15
239	Versatile Coordination Mode of LiNaB8O13 and □and □LiKB8O13 via the Flexible Assembly of Four-Connected B5O10 and B3O7 Groups. *Inorganic Chemistry*, **2016**, 55, 552-4	5.1	15
238	Mo Cation Enrichment of the Structure Chemistry of Iodates: Syntheses, Structures, and Calculations of Ba(MoO)(IO)O, Ba[(MoO)(IO)O(OH)]□2HO, and Sr[(MoO)(IO)O]□HO. *Inorganic Chemistry*, **2018**, 57, 9376-9384	5.1	15
237	Intriguing Structural Transition Inducing Variable Birefringences in ABaMSCl (A = Rb, Cs; M = Ge, Sn). *Inorganic Chemistry*, **2018**, 57, 11310-11313	5.1	15
236	Syntheses, crystal structures, and optical properties of Pb6B3O10X (X=F, Cl, Br). *Journal of Solid State Chemistry*, **2013**, 204, 64-69	3.3	15
235	Evidence of "new hot spots" from determining the nonlinear optical behavior of materials: mechanistic studies of the vanadium borate crystal, Na3VO2B6O11. *Physical Chemistry Chemical Physics*, **2015**, 17, 5338-44	3.6	15
234	Synthesis, crystal structure, and optical properties of a new lead barium borate, PbBa 2 (B 3 O 6) 2. *Journal of Alloys and Compounds*, **2014**, 615, 561-565	5.7	15
233	Guanidinium Fluorooxoborates as Efficient Metal-free Short-Wavelength Nonlinear Optical Crystals. *Chemistry of Materials*, **2022**, 34, 440-450	9.6	15

232	DFT Based Theoretical Study about the Contributions of Fluorine to Nonlinear Optical Properties in Borate Fluoride Crystals. *Crystal Growth and Design*, **2016**, 16, 5067-5073	3.5	15
231	Li6Zn3(BO3)4: a new zincoborate featuring vertex-, edge- and face-sharing LiO4 tetrahedra and exhibiting reversible phase transitions. *Inorganic Chemistry Frontiers*, **2017**, 4, 1100-1107	6.8	14
230	Structure comparison and optical properties of Na7Mg4.5(P2O7)4: a sodium magnesium phosphate with isolated P2O7 units. *New Journal of Chemistry*, **2017**, 41, 3399-3404	3.6	14
229	Alignment of Polar Moieties Leading to Strong Second Harmonic Response in KCsMoP2O9. *Chemistry of Materials*, **2020**, 32, 3297-3303	9.6	14
228	Exploration of a new compound in the MBDX (M: alkali metals; X: halogen) system: Preparation, crystal and electronic structures, and optical properties of Na3B6O10Br. *Inorganica Chimica Acta*, **2013**, 406, 205-210	2.7	14
227	The activity of lone pair contributing to SHG response in bismuth borates: a combination investigation from experiment and DFT calculation. *Physical Chemistry Chemical Physics*, **2017**, 19, 25270-25276	3.6	14
226	Structure, growth and properties of a novel polar material, KSr4B3O9. *Journal of Solid State Chemistry*, **2012**, 195, 73-78	3.3	14
225	Role of the metal cation types around VO4 groups on the nonlinear optical behavior of materials: experimental and theoretical analysis. *Dalton Transactions*, **2016**, 45, 14394-402	4.3	14
224	The Rubidium Barium Borate Resulting from BO Fundamental Building Block Exhibits DUV Cutoff Edge. *Inorganic Chemistry*, **2018**, 57, 13380-13385	5.1	14
223	Combination of d 10 -cations and fluorine anion as active participants to design novel borate/carbonate nonlinear optical materials. *Journal of Alloys and Compounds*, **2018**, 758, 85-90	5.7	14
222	Theoretical investigation on the balance between large band gap and strong SHG response in BMO4 (M = P and As) crystals. *RSC Advances*, **2017**, 7, 2804-2809	3.7	13
221	Design and Synthesis of a Series of Novel Mixed Borate and Carbonate Halides. *Chemistry - A European Journal*, **2017**, 23, 10451-10459	4.8	13
220	The first lithium difluorophosphate LiPOF with a neutral polytetrahedral microporous architecture. *Chemical Communications*, **2019**, 55, 1817-1820	5.8	13
219	Two New Crystals in Li(m)Cs(n)B(m+n)O2(m+n) (m + n = 5, 7; m > n) Series: Noncentrosymmetric Li5Cs2B7O14 and Centrosymmetric Li4CsB5O10. *Inorganic Chemistry*, **2015**, 54, 7381-7	5.1	13
218	Hierarchized band gap and enhanced optical responses of trivalent rare-earth metal nitrates due to (dp)π conjugation interactions. *Journal of Materials Chemistry C*, **2016**, 4, 6295-6301	7.1	13
217	NH4B11O16(OH)2: a new ammonium borate with wavy-shaped polycyclic 2∞[B11O16(OH)2] layers. *New Journal of Chemistry*, **2018**, 42, 12091-12097	3.6	13
216	A new polymorph of Cd3B2O6: synthesis, crystal structure and phase transformation. *RSC Advances* , **2014**, 4, 13195-13200	3.7	13
215	Crystal growth and calculation of the electronic band structure and density of states of Li3Cs2B5O10. *CrystEngComm*, **2014**, 16, 1978	3.3	13

214	Synthesis, crystal structure and properties of a new congruently melting compound, K3ZnB5O10. *Solid State Sciences*, **2012**, 14, 936-940	3.4	13
213	Ba2B6O11, a Member of the BaO-B2O3 Family, Featuring a Layer Framework. *European Journal of Inorganic Chemistry*, **2015**, 2015, 3328-3335	2.3	13
212	Optical Floating Zone Growth of BaB2O4 from a LiBa2B5O10-Based Solvent. *Crystal Growth and Design*, **2007**, 7, 1561-1564	3.5	13
211	RbBOF: a rubidium fluorooxoborate with an unprecedented [BOF] functionalized unit and a large birefringence. *Chemical Communications*, **2020**, 56, 15333-15336	5.8	13
210	"XA6" octahedra influencing the arrangement of anionic groups and optical properties in inverse-perovskite [B6O10]XA3 (X = Cl, Br; A = alkali metal). *Physical Chemistry Chemical Physics*, **2016**, 18, 15394-8	3.6	13
209	Sn2B7O12F with a 2[B14O24]6layer constructed from the unprecedented [B7O16]11 fundamental building block. *Inorganic Chemistry Frontiers*, **2019**, 6, 996-1002	6.8	13
208	BaLiZn3(BO3)3: a new member of the KBe2BO3F2 family possessing dense BO3 triangles and the smallest interlayer distance. *New Journal of Chemistry*, **2018**, 42, 12365-12368	3.6	13
207	The structural diversity of halogen-centered secondary building units: two new mixed-metal borate halides with deep-ultraviolet cut-off edges. *Dalton Transactions*, **2017**, 46, 4923-4928	4.3	12
206	Cation Modulation on the Crystal Structure and Band Gap of Fluorooxoborates ABOF (A = Alkali and Mixed Alkali Metal). *Inorganic Chemistry*, **2019**, 58, 13411-13417	5.1	12
205	Three new phosphates, CsPb(PO), CsLi(PO) and LiCa(PO): structural comparison, characterization and theoretical calculation. *Dalton Transactions*, **2019**, 48, 8948-8954	4.3	12
204	LiNaBO: Featuring Unprecedented BO Fundamental Building Block and Deep-UV Cutoff Edge. *Inorganic Chemistry*, **2018**, 57, 2876-2882	5.1	12
203	KTePO: a new telluro-phosphate with a pentagonal Te-P-O layer structure. *Dalton Transactions*, **2018**, 47, 9453-9458	4.3	12
202	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO3/BO3F Ratio in Layers. *Angewandte Chemie*, **2019**, 131, 11852-11856	3.6	12
201	Na4B8O9F10: ADeep-Ultraviolet Transparent Nonlinear Optical Fluorooxoborate with Unexpected Short Phase-Matching Wavelength Induced by Optimized Chromatic Dispersion.. *Angewandte Chemie - International Edition*, **2021**,	16.4	12
200	Sn PO I: An Excellent Birefringent Material with Giant Optical Anisotropy in Non Conjugated Phosphate. *Angewandte Chemie - International Edition*, **2021**, 60, 24901-24904	16.4	12
199	Application of the dimensional reduction formalism to PbBa[Li(PO)(PO)] (x = 0, 2, 6, 7): a series of phosphates with two types of isolated polyphosphate groups. *Dalton Transactions*, **2017**, 46, 4678-4684	4.3	11
198	ScMO(BO) (M = Ca and Cd): new Sc-based oxyborates featuring interesting edge-sharing sandwich-like chains and UV cut-off edges. *Dalton Transactions*, **2017**, 46, 14839-14846	4.3	11
197	Adjustable optical nonlinearity in d cations containing chalcogenides via dp hybridization interaction. *Dalton Transactions*, **2019**, 48, 2592-2597	4.3	11

196	La B O (OH): The First Acentric High-Pressure Borate Displaying Edge-Sharing BO Tetrahedra. *Chemistry - A European Journal*, **2020**, 26, 6851-6861	4.8	11
195	Crystal Growth and Linear and Nonlinear Optical Properties of KIO3□Te(OH)6. *Crystal Growth and Design*, **2017**, 17, 4405-4412	3.5	11
194	Syntheses, characterization and theoretical studies of three apatite-type phosphates MPb4(PO4)3 (M□= K, Rb, Cs). *Journal of Alloys and Compounds*, **2017**, 690, 330-336	5.7	11
193	Synthesis, crystal structure and optical properties of a new orthorhombic phase, Na3ZnB5O10. *Journal of Molecular Structure*, **2012**, 1021, 118-122	3.4	11
192	LiGeBO4: a nonlinear optical material with a balance between deep-ultraviolet cut-off edge and large SHG response induced by hand-in-hand tetrahedra. *Inorganic Chemistry Frontiers*, **2019**, 6, 914-919	6.8	11
191	Noncentrosymmetric Tetrel Pnictides RuSi4P4 and IrSi3P3: Nonlinear Optical Materials with Outstanding Laser Damage Threshold. *Advanced Functional Materials*, **2021**, 31, 2010293	15.6	11
190	Ba7(BO3)3GeO4X (X = Cl, Br): borogermanate halides with rigid GeO4 tetrahedra and flexible XBa6 octahedra. *RSC Advances*, **2015**, 5, 53448-53454	3.7	10
189	Ba(BOF(OH)) with well-ordered OH/F anions and a unique BOF(OH) dimer. *Chemical Communications*, **2020**, 56, 3301-3304	5.8	10
188	The First Examples of Lithium-Containing Mixed-Alkali Strontium Borates with Different Dimensional Anionic Architectures and Short Cutoff Edges. *Chemistry - A European Journal*, **2018**, 24, 15355-15364	4.8	10
187	The Effect of the Ratio of [M/(B+P)] on the Configuration of Anionic Groups: Synthesis of the Borate□Phosphate LiPb4(BO3)(PO4)2. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3467-3473	2.3	10
186	Linear-to-□Shape P-O-P Bond Transmutation in Polyphosphates with Infinite (PO) Chain. *Inorganic Chemistry*, **2017**, 56, 10139-10142	5.1	10
185	Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angewandte Chemie - International Edition*, **2021**, 60, 10791-10797	16.4	10
184	From silicates to oxonitridosilicates: improving optical anisotropy for phase-matching as ultraviolet nonlinear optical materials. *Chemical Communications*, **2021**, 57, 639-642	5.8	10
183	Two Lanthanide Borate Chlorides LnBO(OH)Cl (Ln = La, Ce) with Wide Ultraviolet Transmission Windows and Large Second-Harmonic Generation Responses. *Inorganic Chemistry*, **2018**, 57, 14953-14960	5.1	10
182	Lone pair effects on ternary infrared nonlinear optical materials. *Physical Chemistry Chemical Physics*, **2019**, 21, 5142-5147	3.6	9
181	From centrosymmetric to noncentrosymmetric: cation-directed structural evolution in X3ZnB5O10 (X = Na, K, Rb) and Cs12Zn4(B5O10)4 crystals. *Inorganic Chemistry Frontiers*, **2019**, 6, 1461-1467	6.8	9
180	Designing Three Fluorooxoborates with a Wide Transmittance Window by Anionic Group Substitution. *Inorganic Chemistry*, **2019**, 58, 3596-3600	5.1	9
179	Three Alkali Metal Lead Orthophosphates □Syntheses, Crystal Structures and Properties of APbPO4 (A = K, Rb, Cs). *European Journal of Inorganic Chemistry*, **2015**, 2015, 1490-1495	2.3	9

178	Synthesis, structures, and properties of two magnesium silicate fluorides Mg5(SiO4)2F2 and Mg3SiO4F2. *New Journal of Chemistry*, **2015**, 39, 8866-8873	3.6	9
177	Noncentrosymmetric Fluorooxoborates ABOF (A = K and Rb) with Unexpected [BOF] Units and Deep-Ultraviolet Cutoff Edges. *Inorganic Chemistry*, **2020**, 59, 3274-3280	5.1	9
176	Coordinated regulation on critical physiochemical performances activated from mixed tetrahedral anionic ligands in new series of SrAMS (A = Ag, Cu; M = Ge, Sn) nonlinear optical materials. *Dalton Transactions*, **2020**, 49, 3388-3392	4.3	9
175	Ba2ZnSc(BO3)3 and Ba4Zn5Sc2(BO3)8: first examples of borates in the ZnScBO system featuring special structure configurations. *Inorganic Chemistry Frontiers*, **2018**, 5, 1787-1794	6.8	9
174	Effect of the tetrahedral groups on the optical properties of LaBRO5 (R = Si and Ge): A first-principles study. *Journal of Applied Physics*, **2015**, 118, 113104	2.5	9
173	Synthesis, structure, and properties of a novel hydrated borate Rb4[B4O5(OH)4]2·H2O. *Solid State Sciences*, **2011**, 13, 82-87	3.4	9
172	Synthesis, crystal structure and optical properties of Li2Cu5(PO4)4. *Solid State Sciences*, **2011**, 13, 1304-1308	3.4	9
171	Unprecedented mid-infrared nonlinear optical materials achieved by crystal structure engineering, a case study of (KX)PS (X = Sb, Bi, Ba).. *Chemical Science*, **2022**, 13, 2640-2648	9.4	9
170	Potential optical functional crystals with large birefringence: Recent advances and future prospects. *Coordination Chemistry Reviews*, **2022**, 459, 214380	23.2	9
169	Effect of anion dimensionality on optical properties: the [BO(OH)] layer in CsBO(OH)vs. the [BO] framework in CsBaBO. *Dalton Transactions*, **2020**, 49, 1292-1299	4.3	9
168	Influence of original and simulated microscopic units on SHG response in semiorganic NLO materials. *RSC Advances*, **2016**, 6, 39534-39540	3.7	9
167	LiRbLaBO: a new rare-earth borate with a MOF-5-like topological structure and a short UV cut-off edge. *Dalton Transactions*, **2016**, 46, 193-199	4.3	8
166	Ligand Engineering for Broadening Infrared Luminescence of Kramers Ytterbium Ions in Disordered Sesquioxides. *Crystal Growth and Design*, **2019**, 19, 3704-3713	3.5	8
165	NaCaBO(SiO) with Interesting Isolated [BO] and [SiO] Units in Alkali- and Alkaline-Earth-Metal Borosilicates. *Inorganic Chemistry*, **2019**, 58, 3937-3943	5.1	8
164	Na3B4O7X (X = Cl, Br): two new borate halides with a 1D Na-X (X = Cl, Br) chain formed by the face-sharing XNa6 octahedra. *RSC Advances*, **2015**, 5, 12416-12422	3.7	8
163	Broadening of the Fluorescence Spectra of Sesquioxide Crystals for Ultrafast Lasers. *Crystal Growth and Design*, **2020**, 20, 4678-4685	3.5	8
162	Polar polymorphism: and KCsWP2O9 nonlinear optical materials with a strong second harmonic generation response. *Journal of Materials Chemistry C*, **2020**, 8, 11441-11448	7.1	8
161	LiBaGaQ (Q = S, Se): Noncentrosymmetric Metal Chalcogenides with a Cesium Chloride Topological Structure Displaying a Remarkable Laser Damage Threshold. *Inorganic Chemistry*, **2020**, 59, 5674-5682	5.1	8

160	The Flexibility of P2O7 Dimers in Soft Structures: M2CdP2O7 (M = Rb, Cs). *European Journal of Inorganic Chemistry*, **2016**, 2016, 2704-2708	2.3	8
159	Flexible coordination of Pb atoms and variable zinc–borate frameworks to construct three Pb5Zn4B6O18 polymorphs. *Inorganic Chemistry Frontiers*, **2018**, 5, 2501-2507	6.8	8
158	Experiment and First-Principles Calculations of AMgTeBO (A = Pb, Ba): Influences of the Cosubstitution on the Structure Transformation and Optical Properties. *Inorganic Chemistry*, **2019**, 58, 11127-11132	5.1	8
157	Reinvestigation and Characterization of the Magnesium Borate Fluoride Mg5(BO3)F. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2014**, 640, 2013-2018	1.3	8
156	A new cesium pentaborate with new B10O19 building blocks. *Inorganic Chemistry*, **2014**, 53, 2358-60	5.1	8
155	Synthesis, Crystal Structure, and Properties of a New Lead Barium Borate, Pb1.13Ba7.87B18O36. *Chemistry Letters*, **2012**, 41, 812-813	1.7	8
154	NaPN2: Deep-ultraviolet nonlinear optical material with unprecedented strong second-harmonic generation coefficient. *Physical Review Materials*, **2019**, 3,	3.2	8
153	Insights of BO3–PO4 replacement for the design and synthesis of a new borate–phosphate with unique 1[Zn4BO11] chains and two new phosphates. *Inorganic Chemistry Frontiers*, **2018**, 5, 327-334	6.8	8
152	NaRbBO(OH)(HCO): A Borate-Bicarbonate Nonlinear Optical Material. *Inorganic Chemistry*, **2020**, 59, 759-766	5.1	8
151	CsBOF with a Deep-Ultraviolet Cutoff Edge and a Suitable Birefringence as the Potential Zero-Order Waveplate Material. *Inorganic Chemistry*, **2020**, 59, 13014-13018	5.1	8
150	SnF2: A UV Birefringent Material with Large Birefringence and Easy Crystal Growth. *Angewandte Chemie*, **2021**, 133, 3582-3586	3.6	8
149	First-principles study lone-pair effects of Sb (III)-S chromophore influence on SHG response in quaternary potassium containing silver antimony sulfides. *Journal of Solid State Chemistry*, **2017**, 249, 215-220	3.3	7
148	DFT-Based Comparative Study about the Influence of Fluorine and Hydroxyl Anions on Opto-Electric Properties of Borate Crystals: Choice for Better Anion. *Inorganic Chemistry*, **2017**, 56, 5636-5645	5.1	7
147	Na2ZnSn2S6: A mixed-metal thiostannate with large second-harmonic generation response activated by penta-tetrahedral [ZnSn4S14]10 clusters. *Science China Technological Sciences*, **2017**, 60, 1465-1472	3.5	7
146	CO(NH2)2 NH4Cl: an ultraviolet birefringent material with conjugated CO groups. *CrystEngComm*, **2019**, 21, 6072-6079	3.3	7
145	K[BO(OH)](CO)X 7HO (X = Cl, Br): Syntheses, Characterizations, and Theoretical Studies of Noncentrosymmetric Halogen Borate-Carbonates with Short UV Cutoff Edges. *Inorganic Chemistry*, **2019**, 58, 6974-6982	5.1	7
144	Cs2Zn5(PO4)4 and Cs3La(PO4)2: Two Cs-Containing Phosphates with Three-Dimensional Frameworks. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2462-2467	2.3	7
143	LiCaBO: A Borate with a Unique Fundamental Building Block and a Short Cutoff Edge. *Inorganic Chemistry*, **2020**, 59, 8396-8403	5.1	7

142	Structural Diversity of Molybdate Iodate and Fluoromolybdate: Syntheses, Structures, and Calculations on Na(MoO)(IO) and NaCs(MoOF). *Inorganic Chemistry*, **2020**, 59, 3034-3041	5.1	7
141	M2Ca3B16O28 (M = Rb, Cs): structures analogous to SBBO with three-dimensional open-framework layers. *RSC Advances*, **2016**, 6, 14205-14210	3.7	7
140	Research and Development of Zincoborates: Crystal Growth, Structural Chemistry and Physicochemical Properties. *Molecules*, **2019**, 24,	4.8	7
139	Ba3Ca4(BO3)3(SiO4)Cl: a new non-centrosymmetric complex alkaline-earth metal borosilicate chloride with a deep-ultraviolet cut-off edge. *Inorganic Chemistry Frontiers*, **2019**, 6, 2200-2208	6.8	7
138	BaBOF□0.1KF: the first mixed alkali/alkaline-earth metal fluorooxoborate with unprecedented double-layered B-O/F anionic arrangement. *Chemical Communications*, **2019**, 55, 8923-8926	5.8	7
137	Two new ammonium/alkali-rare earth metal difluorophosphates ALa(POF) (A = NH and K) with moderate birefringence and short cutoff edges. *Dalton Transactions*, **2020**, 49, 11591-11596	4.3	7
136	Unique Unilateral-Chelated Mode-Induced d□□nteraction Enhances Second-Harmonic Generation Response in New Ln3LiMS7 Family. *Chemistry of Materials*, **2021**, 33, 4225-4230	9.6	7
135	Cs B O F : First Fluorooxoborate with [BF] Involving Heteroanionic Units and Extremely Low Melting Point. *Chemistry - A European Journal*, **2021**, 27, 9753-9757	4.8	7
134	Centrosymmetric or Noncentrosymmetric? Transition Metals Talking in KTGeS(T = Co, Fe). *Inorganic Chemistry*, **2021**, 60, 10603-10613	5.1	7
133	Li BaSc(BO) F and LiBa Pb(BO) F with Layered Structures featuring Special Li-O/F Configurations. *Chemistry - A European Journal*, **2018**, 24, 15477-15481	4.8	7
132	CsBaB9O15: a high performance ultraviolet nonlinear optical material activated by the peculiar double layered configuration. *Science Bulletin*, **2021**, 66, 2165-2169	10.6	7
131	A series of MPS (M = Ag, Cu and Ag/Cu) thiophosphates with diamond-like structures exhibiting large second harmonic generation responses and moderate ion conductivities. *Dalton Transactions*, **2021**, 50, 4129-4132	4.3	7
130	Experimental and ab initio studies of two UV nonlinear optical materials. *RSC Advances*, **2017**, 7, 20259-20265	3.7	6
129	Prediction of ternary fluorooxoborates with coplanar triangular units [BOF] from first-principles. *Dalton Transactions*, **2020**, 49, 5424-5428	4.3	6
128	Synthesis, Crystal Structures, Optical Properties and Theoretical Calculations of Two Metal Chalcogenides Ba2AlSbS5 and Ba2GaBiSe5. *Crystals*, **2018**, 8, 165	2.3	6
127	A new barium-containing alkali metal silicate fluoride NaBa3Si2O7F with deep-UV optical property. *Science China Materials*, **2019**, 62, 1454-1462	7.1	6
126	Ba2In2Q5 (Q = S, Se): Synthesis, Crystal Structures, Electronic Structures, and Optical Properties. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 1329-1333	1.3	6
125	One-Dimensional Double Chains in Sodium-Based Quaternary Chalcogenides Displaying Intriguing Red Emission and Large Optical Anisotropy. *Inorganic Chemistry*, **2020**, 59, 2519-2526	5.1	6

124	K(POF)(SO): first fluorooxophosphorsulfate with mixed-anion [SO] and [POF] groups. *Dalton Transactions*, **2020**, 49, 17658-17664	4.3	6
123	Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angewandte Chemie*, **2021**, 133, 10886-10892	3.6	6
122	Computationally assisted multistage design and prediction driving the discovery of deep-ultraviolet nonlinear optical materials. *Materials Chemistry Frontiers*, **2021**, 5, 3507-3523	7.8	6
121	Noncentrosymmetric Rare-Earth Borate Fluoride LaBOF: A New Ultraviolet Nonlinear Optical Crystal with Enhanced Linear and Nonlinear Performance.. *ACS Applied Materials & Interfaces*, **2022**,	9.5	6
120	□-Pb4B2O7 and □-Pb4B6O13: Polymorphism drives changes in structure and performance. *Science China Materials*, **2020**, 63, 806-815	7.1	5
119	A Promising Fluorooxoborate Framework with Flexibile Capability for Diverse Cations to Enhance the Second Harmonic Generation. *Chemistry - A European Journal*, **2020**, 26, 3723-3728	4.8	5
118	New fluoroborate Cd8B5O15F with two different isolated borate anions prepared by an open high-temperature solution method. *Dalton Transactions*, **2016**, 45, 7008-13	4.3	5
117	Two noncentrosymmetric polyphosphates featuring infinite one-dimensional (PO3)□chain, LiMP2O6 (M = Rb, Cs): Synthesis, structure and optical properties. *Journal of Solid State Chemistry*, **2018**, 266, 150-154	3.3	5
116	Four alkali metal molybdates with two types of MoO chains, ABMo3O10 (A = Li, B = Rb; A = Li, Na, K, B = Cs): synthesis, structure comparison and optical properties. *New Journal of Chemistry*, **2018**, 42, 10879-10884	3.6	5
115	Structural insights into three phosphates with distinct polyanionic configurations. *Dalton Transactions*, **2019**, 48, 13406-13412	4.3	5
114	Sr8MB18O36 (M = Zn or Cd): Design and Synthesis of Two New Borates with a Special Ratio of 8:1. *Chemistry Letters*, **2014**, 43, 1216-1218	1.7	5
113	Synthesis and characterization of two lead-containing metal chalcogenides: Ba5Pb2Sn3S13 and Ba6PbSn3Se13. *Journal of Solid State Chemistry*, **2017**, 255, 133-138	3.3	5
112	Achieving Short-Wavelength Phase-Matching Second Harmonic Generation in Boron-Rich Borosulfate with Planar [BO] Units. *Angewandte Chemie - International Edition*, **2021**,	16.4	5
111	Enhanced optical anisotropy dimensional control in alkali-metal chalcogenides. *Physical Chemistry Chemical Physics*, **2020**, 22, 19697-19703	3.6	5
110	Three non-centrosymmetric bismuth phosphates, Li2ABi(PO4)2 (A = K, Rb, and Cs): effects of cations on the crystal structure and SHG response. *Inorganic Chemistry Frontiers*, **2020**, 7, 3364-3370	6.8	5
109	Intense d-p Hybridization Induced a Vast SHG Response Disparity between Tetrahedral Vanadates and Arsenates. *Journal of Physical Chemistry C*, **2020**, 124, 24949-24956	3.8	5
108	Ba (BO)(CO)F: The First Borate Carbonate Fluoride Synthesized by the High-Temperature Solution Method. *Chemistry - A European Journal*, **2020**, 26, 16628-16632	4.8	5
107	Pb3Ba7B7O20F: A new nonlinear optical material exhibiting large second harmonic generation response induced by its unprecedented Pb-B-O framework. *Scripta Materialia*, **2021**, 194, 113700	5.6	5

106	M3B6O10NO3 (M = K, Rb): Two New Alkali Metal Borate-Nitrates with Noncentrosymmetric Structures. *European Journal of Inorganic Chemistry*, **2021**, 2021, 1297-1304	2.3	5
105	Manipulation of birefringence via substitution of Sr2+ by Pb2+ based on the structure model of LiSr1−xPbxBO3 (0 ≤ x ≤ 0.5). *New Journal of Chemistry*, **2016**, 40, 6120-6126	3.6	5
104	Ba(BSS)S: a new thioborate with unprecedented [BS-S] and [S] fundamental building blocks. *Chemical Communications*, **2019**, 55, 14793-14796	5.8	5
103	Ba2B7O12F with novel FBB [B7O16F] and deep-ultraviolet cut-off edge. *Inorganic Chemistry Frontiers*, **2021**, 8, 339-343	6.8	5
102	NaBaMQ (M = Al, Ga; Q = S, Se): first quaternary chalcogenides with isolated edge-sharing (MQ) dimers. *Dalton Transactions*, **2018**, 47, 16044-16047	4.3	5
101	Ion-induced structural and optical performance evolution in LBO-like crystals: experimental and theoretical investigation. *Inorganic Chemistry Frontiers*, **2018**, 5, 2955-2963	6.8	5
100	Finding the First Squarates Nonlinear Optical Crystal NaHC4O4·H2O with Strong Second Harmonic Generation and Giant Birefringence **2022**, 4, 572-576		5
99	LiMCO (M = K, Rb, Cs): a series of mixed alkali carbonates with large birefringence. *Dalton Transactions*, **2017**, 46, 6894-6899	4.3	4
98	LiBaMQ (M = Al, Ga, In; Q = S, Se): A Series of Metal Chalcogenides with a Structural Transition. *Inorganic Chemistry*, **2019**, 58, 12859-12866	5.1	4
97	RbBaTeBO: a novel [BO] fundamental building block in a new telluroborate with [TeO] polyhedra. *Dalton Transactions*, **2020**, 49, 8911-8917	4.3	4
96	Controllable synthesis and spontaneous phase transition of photonic coordination polymer to produce a strong second-harmonic generation response. *Science China Materials*, **2020**, 63, 1272-1278	7.1	4
95	LiCsLa(BO) and LiKLa(BO): new mixed alkali metal lanthanum borates with three-dimensional open frameworks and short cut-off edges. *Dalton Transactions*, **2018**, 47, 3512-3520	4.3	4
94	Nonlinear optical response mechanism of noncentrosymmetric lead borate Pb6[B4O7(OH)2]3 with three crystallographically independent [B4O7(OH)2]4− chains. *RSC Advances*, **2016**, 6, 100849-100856	3.7	4
93	A Fluorooxosilicophosphate with an Unprecedented SiO2F4 Species. *Angewandte Chemie*, **2018**, 130, 9976-9980	3.6	4
92	Synthesis, crystal structure and optical properties of a new lithium dilead pentaborate, LiPb2B5O10. *Journal of Molecular Structure*, **2013**, 1040, 180-183	3.4	4
91	NaSiSO: the first example of a sulfide silicate exhibiting unusual tri-polymerized [SiSO] units without S-O bonds. *Dalton Transactions*, **2017**, 46, 13356-13359	4.3	4
90	SrNO3(OH)·H2O: A new member in strontium nitrate hydrate family with an ultraviolet cut-off edge. *Journal of Alloys and Compounds*, **2017**, 695, 1719-1724	5.7	4
89	Synthesis-enabled exploration of chiral and polar multivalent quaternary sulfides. *Chemical Science*, **2021**, 12, 14718-14730	9.4	4

88	Al(BO)(BO)F: A F-Containing Aluminum Borate Featuring Two Types of Isolated B-O Groups. *Inorganic Chemistry*, **2020**, 59, 810-817	5.1	4
87	Discovery of First Magnesium Fluorooxoborate with Stable Fluorine Terminated Framework for Deep-UV Nonlinear Optical Application. *Angewandte Chemie*, **2021**, 133, 14771-14777	3.6	4
86	RbMT (BO) O (M=Ba, Sr; T=Al, Ga): New Double-Layered Oxyborates Constructed from [BO] Triangles and [TO] Tetrahedra. *Chemistry - A European Journal*, **2021**, 27, 8698-8703	4.8	4
85	Density functional theory calculations, growth, structure, and optical properties of birefringent LiNaV2O6. *Journal of Materials Research*, **2016**, 31, 488-494	2.5	4
84	Mg(HO)BO(OH)(HO): a new hydrated borate with a short DUV cutoff edge. *Dalton Transactions*, **2019**, 48, 17408-17413	4.3	4
83	Barium fluoroiodate crystals with a large band gap and birefringence. *Inorganic Chemistry Frontiers*,	6.8	4
82	BaBSCl and BaBSCl: first alkaline-earth metal thioborate halides with [BS] units. *Chemical Communications*, **2021**, 57, 6440-6443	5.8	4
81	An antimony(III) borate with large birefringence exhibiting unwonted [B5O11] fundamental building blocks and dimeric [Sb2O6] clusters. *Inorganic Chemistry Frontiers*, **2021**, 8, 2584-2590	6.8	4
80	Tetrafluoroborate-Monofluorophosphate (NH4)3[PO3F][BF4]: First Member of Oxyfluoride with B F and P F Bonds. *ACS Organic & Inorganic Au*,		4
79	Li4MgGe2S7: The First Alkali and Alkaline-Earth Diamond-Like Infrared Nonlinear Optical Material with Exceptional Large Band Gap. *Angewandte Chemie*,	3.6	4
78	Toward the Rational Design of Mid-Infrared Nonlinear Optical Materials with Targeted Properties via a Multi-Level Data-Driven Approach. *Advanced Functional Materials*,2200231	15.6	4
77	The Combination of Structure Prediction and Experiment for the Exploration of Alkali-Earth Metal-Contained Chalcopyrite-Like IR Nonlinear Optical Material.. *Advanced Science*, **2022**, e2106120	13.6	4
76	From oxides to oxysulfides: the mixed-anion GeS3O unit induces huge improvement in the nonlinear optical effect and optical anisotropy for potential nonlinear optical materials. *RSC Advances*, **2022**, 12, 16296-16300	3.7	4
75	Syntheses, crystal structures and characterization of three alkaline metal borates. *CrystEngComm*, **2017**, 19, 2561-2569	3.3	3
74	[Ge S (S)] , A NLO-Active Unit Leading to an Asymmetric Structure Discovered in Li Cs Ge S (S)Cl : An Experimental and Theoretical study. *Chemistry - A European Journal*, **2019**, 25, 5440-5444	4.8	3
73	Active performance of tetrahedral groups to SHG response: theoretical interpretations of Ge/Si-containing borate crystals. *Physical Chemistry Chemical Physics*, **2016**, 18, 6077-84	3.6	3
72	Structural modulation induced by M metals in BaMQX (M = Al, Ga, In; Q = S, Se; X = Cl, Br): an experimental and computational analysis. *Dalton Transactions*, **2019**, 48, 12713-12719	4.3	3
71	BaPbSi2O6 BaSO4: the first mixed anionic compound synthesized via BaSO4 salt-inclusion. *CrystEngComm*, **2014**, 16, 5993-5996	3.3	3

70	Preparation, Structure, and Second-order Nonlinear Optical Properties of a Borate-Carboxylic Acid Compound: NH4B[d-(+)-C4H4O5]2·H2O. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2014**, 640, 140-146	1.3	3
69	Ba2Cd(B3O6)2: A Congruent-Melting Compound with Isolated B3O6 Units. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 988-993	1.3	3
68	Polymorphic Pb14O8I12 and Pb7O4I6 oxyhalides featuring unprecedented [O8Pb14] clusters with broad IR transparency. *Science China Materials*,1	7.1	3
67	Role of Fluorooxo-Functional Units in Symmetry Breaking and Second Harmonic Generation Response Contribution in Fluorooxoborate Nonlinear Optical Crystals. *Crystal Growth and Design*, **2020**, 20, 7582-7587	3.5	3
66	Na MQ (M=Zn, Cd; Q=S, Se): Promising New Ternary Infrared Nonlinear Optical Materials. *Chemistry - A European Journal*, **2021**, 27, 6538-6544	4.8	3
65	Cation Substitution of Hexagonal Triple Perovskites: A Case in Trimetallic Tellurates AA'BTeO. *Inorganic Chemistry*, **2021**, 60, 6099-6106	5.1	3
64	Yb:GdScO crystal for efficient ultrashort pulse lasers. *Optics Letters*, **2021**, 46, 3641-3644	3	3
63	A 119Sn M□sbauer-spectroscopic characterization of the diamagnetic birefringence material Sn2B5O9Cl. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2019**, 74, 879-883	1	3
62	Three diphosphates, □LiNaPO, LiPbBa(PO) and LiRb(PO): influences of co-substitution on the crystal structure. *Dalton Transactions*, **2020**, 49, 6744-6750	4.3	3
61	Series of Crystals with Giant Optical Anisotropy: A Targeted Strategic Research. *Angewandte Chemie*, **2021**, 133, 1352-1358	3.6	3
60	CsAlBO: a short-wavelength nonlinear optical crystal with moderate second harmonic generation response. *Dalton Transactions*, **2021**, 50, 822-825	4.3	3
59	Sn14O11Br6: a promising birefringent material with a [Sn14O11Br6] layer. *Journal of Materials Chemistry C*, **2021**, 9, 7103-7109	7.1	3
58	Synergism of multiple functional chromophores significantly enhancing the birefringence in layered non-centrosymmetric chalcohalides. *Inorganic Chemistry Frontiers*, **2021**, 8, 1588-1598	6.8	3
57	BaTi(BO3)2: an excellent birefringent material with highly coplanar isolated [BO3] groups. *New Journal of Chemistry*, **2021**, 45, 7065-7068	3.6	3
56	Na4SnS4 and Na4SnSe4 exhibiting multifunctional physicochemical performances as potential infrared nonlinear optical crystals and sodium ion conductors. *New Journal of Chemistry*, **2021**, 45, 12362-12366	3.6	3
55	Finding Short-Wavelength Birefringent Crystals with Large Optical Anisotropy Activated by □Conjugated [C(NH2)3] Units. *Crystal Growth and Design*, **2021**, 21, 1869-1877	3.5	3
54	Hydroxyfluorooxoborate Na[B3O3F2(OH)2]?[B(OH)3]: Optimizing the Optical Anisotropy with Heteroanionic Units for Deep Ultraviolet Birefringent Crystals. *Angewandte Chemie*, **2021**, 133, 20632-20638	3.6	3
53	Rb5Ba2(B10O17)2(BO2): The formation of unusual functional [BO2]□ in borates with deep-ultraviolet transmission window. *Science China Chemistry*, **2022**, 65, 719-725	7.9	3

52	[C3N6H7]2[B3O3F4(OH)]: a new hybrid birefringent crystal with strong optical anisotropy induced by mixed functional units. *Journal of Materials Chemistry C*,	7.1	3
51	K2[B4O5(OH)4]·H2O and K2[B4O5(OH)4]: two new hydrated potassium borates with isolated [B4O5(OH)4]2− units and different structural frameworks. *New Journal of Chemistry*, **2019**, 43, 11660-11665	3.6	2
50	Two alkali calcium borates exhibiting second harmonic generation and deep-UV cutoff edges. *New Journal of Chemistry*, **2019**, 43, 9354-9363	3.6	2
49	BaGeO: A Mid-IR Transparent Crystal with Superstrong Raman Response. *Inorganic Chemistry*, **2020**, 59, 3542-3545	5.1	2
48	Band-Gap Modulation of Nonlinear-Optical Fluorooxoborates by Controlling the F/B Ratios. *Inorganic Chemistry*, **2020**, 59, 1588-1591	5.1	2
47	Hydrogen Bonding Behaviors in Inorganic Solids. *Reviews in Advanced Sciences and Engineering*, **2012**, 1, 75-86		2
46	From ÊNa B O to Na AlB O and Na Al B O : Structural Tuning of Anionic-Group Architectures by Substitution of [BO] by [AlO] Covalent Tetrahedra. *Chemistry - A European Journal*, **2021**,	4.8	2
45	Syntheses, Structures and Properties of Alkali and Alkaline Earth Metal Diamond-Like Compounds LiMgMSe (M = Ge, Sn). *Materials*, **2021**, 14,	3.5	2
44	SnBO: A Ternary Tin(II) Borate with Flexible [BO] Fundamental Building Block Formed by [BO] and [BO] Groups. *Inorganic Chemistry*, **2021**, 60, 883-891	5.1	2
43	Triclinic Layered AZnSiS (A = Rb and Cs) with Large Optical Anisotropy and Systematic Research on the Inherent Structure-Performance Relationship in the AMMQ Family. *Inorganic Chemistry*, **2021**, 60, 12573-12579	5.1	2
42	Na3AMg7(PO4)6 (A = K, Rb and Cs): Structures, properties and theoretical studies of alkali metal magnesium orthophosphates. *Journal of Molecular Structure*, **2021**, 1226, 129349	3.4	2
41	BaPbBO: structural transformation from a centrosymmetric to a noncentrosymmetric space group by introducing Pb into BaBO. *Dalton Transactions*, **2021**, 50, 13031-13036	4.3	2
40	From borophosphate to fluoroborophosphate: a rational design of fluorine-induced birefringence enhancement. *Science China Chemistry*, **2021**, 64, 1498-1503	7.9	2
39	Identical in Formula but Not Isotypic in Configuration: Discovery of a New Highly Polymerized [BO] Cluster in CsAlBO. *Inorganic Chemistry*, **2021**, 60, 15131-15135	5.1	2
38	BaBOF with reversible phase transition featuring unprecedented fundamental building blocks of [BOF] in the -phase and [BOF] in the -phase. *Chemical Communications*, **2021**, 57, 4182-4185	5.8	2
37	LiB5O5F2(OH)4: A new deep-ultraviolet birefringent crystal with [B5O5F2(OH)4] anionic group. *Science China Materials*,1	7.1	2
36	BeCOF Monolayer: A Flexible Ultraviolet Nonlinear Optical Material via Rational Design. *Inorganic Chemistry*, **2019**, 58, 7715-7721	5.1	1
35	The first barium lead oxychloride Ba27Pb8O8Cl54 with new isolated [Pb4O4] clusters. *Journal of Molecular Structure*, **2019**, 1190, 23-28	3.4	1

34	From BaAl2(BO3)2O to SnAl2(BO3)2F2: structure transformation based on ion regulation. *New Journal of Chemistry*, **2020**, 44, 9852-9857	3.6	1
33	Syntheses, structures, and characterization of two new rubidium cadmium(II)/zinc(II) borates: Rb3MB5O10 (M = Cd, Zn). *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2013**, 228,	1	1
32	1.21-W 532-nm picosecond green laser generated by second-harmonic generation using K3B6O10Cl as a nonlinear optical crystal. *Optical Engineering*, **2018**, 57, 1	1.1	1
31	Fluorooxoborate layers: second harmonic generation and Raman spectra anisotropy. *New Journal of Chemistry*, **2020**, 44, 13939-13943	3.6	1
30	LiLa(BO) and LiNaLa(BO): A Great Enhancement in Birefringence Induced by Optimal Arrangement of Conjugated [BO] Units. *Inorganic Chemistry*, **2021**, 60, 12565-12572	5.1	1
29	AB11O16(OH)2 (A = K and Cs): interpenetrating 2D layers with large birefringence. *CrystEngComm*, **2021**, 23, 35-39	3.3	1
28	From thiophosphate to chalcohalide: mixed-anion AgSCl ligands concurrently enhancing nonlinear optical effects and laser-damage threshold. *Chemical Communications*, **2021**, 57, 8218-8221	5.8	1
27	BaZn(BO)F: a new beryllium-free zincoborate with a KBBF-type structure. *Dalton Transactions*, **2021**, 50, 13216-13219	4.3	1
26	SrTi(IO)2HO and SrSn(IO): distinct arrangements of lone pair electrons leading to large birefringences.. *RSC Advances*, **2021**, 11, 10309-10315	3.7	1
25	From centrosymmetric to noncentrosymmetric: effect of the cation on the crystal structures and birefringence values of (NH)AE(POF) (AE = Mg, Sr and Ba; = 2, 3 and 4). *Dalton Transactions*, **2021**, 50, 10206-10213	4.3	1
24	From BaCl2 to Ba(NO3)Cl: significantly enhanced birefringence derived from conjugated [NO3]. *New Journal of Chemistry*, **2021**, 45, 17544-17550	3.6	1
23	Pb2.28Ba1.72B10O19 featuring a three-dimensional BO anionic network with edge-sharing [BO4] obtained under ambient pressure. *Inorganic Chemistry Frontiers*, **2021**, 8, 3716-3722	6.8	1
22	BaBOBr: a new barium borate halide with B-O layered structure. *Dalton Transactions*, **2018**, 47, 16418-16421	4.3	1
21	Two deep-ultraviolet nonlinear optical monolayers obtained by a template-optimized design strategy. *Inorganic Chemistry Frontiers*,	6.8	1
20	Removing Center An Effective Structure Design Strategy for Nonlinear Optical Crystals. *Chemistry of Materials*, **2022**, 34, 2429-2438	9.6	1
19	Lone Pair-Driven Enhancement of Birefringence in Polar Alkali Metal Antimony Phosphates. *Chemistry of Materials*, **2022**, 34, 4224-4231	9.6	1
18	An alkali metal phosphate RbPbBi2(PO4)3 with three kinds of disorder: the effect of isolated soft cation units on the crystal structure. *Inorganic Chemistry Frontiers*, **2019**, 6, 2050-2054	6.8	0
17	AZn2(BO3)Si2O5 (A = Rb, Cs): first examples of KBe2BO3F2 structure type in the borosilicate family exhibiting a deep-ultraviolet cutoff edge. *Journal of Materials Chemistry C*, **2022**, 10, 1727-1734	7.1	0

16	Pd and octahedra do not get along: Square planar [PdS4] units in non-centrosymmetric La6PdSi2S14. *Journal of Alloys and Compounds*, **2022**, 902, 163756	5.7	0
15	Design of a diamond-like infrared nonlinear optical material LiBS2 with ultra-wide band gap. *Journal of Alloys and Compounds*, **2022**, 902, 163839	5.7	0
14	Ba2B13O19(OH)5□5H2O: A promising nonlinear optical material with a unique 2[B13O19(OH)5]□ two-dimensional layer. *Journal of Alloys and Compounds*, **2022**, 897, 163194	5.7	0
13	Na+/Ag+ substitution induced birefringence enhancement from AgGaS2 to NaGaS2. *Journal of Alloys and Compounds*, **2022**, 896, 163093	5.7	0
12	Rational combination of multiple structural groups on regulating nonlinear optical property in hexagonal Ln3MGeS7 polar crystals. *Journal of Alloys and Compounds*, **2022**, 900, 163535	5.7	0
11	A new broad-band infrared window material CdPbOCl with excellent comprehensive properties. *Dalton Transactions*, **2021**, 50, 16401-16405	4.3	0
10	The First Mixed Calcium Zinc Borate with a Flexible [B O] Fundamental Building Block and Short UV Cutoff Edge. *Chemistry - A European Journal*, **2021**, 27, 12047-12051	4.8	0
9	Design and synthesis of BaSiSe with suitable birefringence modulated via M atoms in the Ba-M-Q (M = Si, Ge; Q = S, Se) system. *Dalton Transactions*, **2021**, 50, 11999-12005	4.3	0
8	NaRbB O F : A New Fluorooxoborate with a Short UV Cutoff Edge Enriching the Structural Chemistry of Borate. *Chemistry - an Asian Journal*, **2021**, 16, 3082-3085	4.5	0
7	Sn2PO4I: An Excellent Birefringent Material with Giant Optical Anisotropy in Non□Conjugated Phosphate. *Angewandte Chemie*, **2021**, 133, 25105	3.6	0
6	Sr5(CO3)2(BO3)2: A new family member of isostructural mixed borate and carbonate Ba4M(BO3)2(CO3)2 (M = Ba, Sr) with isolated BO3 and CO3 groups. *Journal of Molecular Structure*, **2022**, 1247, 131382	3.4	0
5	Innenrücktitelbild: SrB5O7F3 Functionalized with [B5O9F3]6□Chromophores: Accelerating the Rational Design of Deep-Ultraviolet Nonlinear Optical Materials (Angew. Chem. 21/2018). *Angewandte Chemie*, **2018**, 130, 6461-6461	3.6	
4	Achieving Short-Wavelength Phase-Matching Second Harmonic Generation in Boron-Rich Borosulfate with Planar [BO3] Units. *Angewandte Chemie*, **2022**, 134, e202112844	3.6	
3	Ce(IO3)2F2?H2O: The First Rare-Earth-Metal Iodate Fluoride with Large Second Harmonic Generation Response. *Chemistry - A European Journal*, **2019**, 25, 1116-1116	4.8	
2	The synthesis, characterization, and theoretical analysis of (NH4)3PbCl5. *New Journal of Chemistry*, **2021**, 45, 2038-2043	3.6	
1	Innenrücktitelbild: Li4MgGe2S7: The First Alkali and Alkaline-Earth Diamond-Like Infrared Nonlinear Optical Material with Exceptional Large Band Gap (Angew. Chem. 45/2021). *Angewandte Chemie*, **2021**, 133, 24535	3.6	