

Lei Kang

List of Publications by Year in descending order

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105
papers

5,801
citations

76196

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76769

74
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120
all docs

120
docs citations

120
times ranked

3189
citing authors

#	ARTICLE	IF	CITATIONS
1	Tourmaline with ultraviolet optical nonlinearity: Emergent material discovery from mineral. Journal of Alloys and Compounds, 2022, 892, 162235.	2.8	2
2	Role of interlayer coupling in second harmonic generation in bilayer transition metal dichalcogenides. Physical Review B, 2022, 105, .	1.1	9
3	Sliding Modulation in Nonlinear Optical Effect in Two-Dimensional van der Waals Cu_2MoS_4 . ACS Applied Materials & Interfaces, 2022, 14, 9535-9543.	4.0	5
4	Surface functionalization of phosphorene via P-H bond for ambient protection and robust photocatalytic H ₂ evolution. Science China Materials, 2022, 65, 1245-1251.	3.5	2
5	Mid-Infrared Nonlinear Optical Halides with Diamond-like Structures: A Theoretical and Experimental Study. Chemistry of Materials, 2022, 34, 5301-5310.	3.2	9
6	Deep-ultraviolet nonlinear optical crystals: concept development and materials discovery. Light: Science and Applications, 2022, 11, .	7.7	55
7	Nonlinear Optical Oxythiophosphate Approaching the Good Balance with Wide Ultraviolet Transparency, Strong Second Harmonic Effect, and Large Birefringence. Angewandte Chemie, 2021, 133, 6456-6460.	1.6	12
8	Nonlinear Optical Oxythiophosphate Approaching the Good Balance with Wide Ultraviolet Transparency, Strong Second Harmonic Effect, and Large Birefringence. Angewandte Chemie - International Edition, 2021, 60, 6386-6390.	7.2	49
9	Electrochemical ammonia synthesis from nitrite assisted by <i>in situ</i> generated hydrogen atoms on a nickel phosphide catalyst. Chemical Communications, 2021, 57, 7176-7179.	2.2	18
10	Regulating Guanidinium-Based Hybrid Materials for Ultraviolet Nonlinear Optical Applications by Hybrid Strength and Hybrid Pattern. Inorganic Chemistry, 2021, 60, 3834-3842.	1.9	16
11	Alloy Engineering of a Polar $(\text{Si,Ge})_2\text{N}_2\text{O}$ System for Controllable Second Harmonic Performance. Inorganic Chemistry, 2021, 60, 7381-7388.	1.9	5
12	Second harmonic generation of $\text{Mo}_4\text{Si}_2\text{N}_4$ -type layers. Physical Review B, 2021, 103, .	1.1	20
13	$\text{LiZn}(\text{OH})\text{CO}_3$: A Deep-Ultraviolet Nonlinear Optical Hydroxycarbonate Designed from a Diamond-like Structure. Angewandte Chemie - International Edition, 2021, 60, 13574-13578.	7.2	88
14	$\text{LiZn}(\text{OH})\text{CO}_3$: A Deep-Ultraviolet Nonlinear Optical Hydroxycarbonate Designed from a Diamond-like Structure. Angewandte Chemie, 2021, 133, 13686-13690.	1.6	9
15	Deep-Ultraviolet Nonlinear Optical van der Waals Beryllium Borates**. Angewandte Chemie - International Edition, 2021, 60, 16680-16686.	7.2	17
16	Deep-Ultraviolet Nonlinear Optical van der Waals Beryllium Borates**. Angewandte Chemie, 2021, 133, 16816-16822.	1.6	4
17	Fluorine Effects for Tunable C-C and C-S Bond Cleavage in Fluoro-Julia-Kocienski Intermediates. CCS Chemistry, 2021, 3, 1678-1689.	4.6	4
18	Novel van der Waals Deep-UV Nonlinear Optical Materials. Chemistry - A European Journal, 2021, 27, 17269-17272.	1.7	1

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19	Two metal-free cyanurate crystals with a large optical birefringence resulting from the combination of π -conjugated units. Dalton Transactions, 2021, 50, 17495-17498.	1.6	5
20	First-Principles Design and Simulations Promote the Development of Nonlinear Optical Crystals. Accounts of Chemical Research, 2020, 53, 209-217.	7.6	194
21	Realizing Deep-Ultraviolet Second Harmonic Generation by First-Principles-Guided Materials Exploration in Hydroxyborates. Journal of the American Chemical Society, 2020, 142, 15157-15163.	6.6	66
22	Layered oxide SBO_2 with a deep-ultraviolet band gap and a strong and robust second-harmonic generation. Physical Review B, 2020, 101, 114103.	1.1	25
23	Anomalous mechanical materials squeezing three-dimensional volume compressibility into one dimension. Nature Communications, 2020, 11, 5593.	5.8	19
24	Deep-ultraviolet nonlinear optical crystals by design: A computer-aided modeling blueprint from first principles. Science China Materials, 2020, 63, 1597-1612.	3.5	33
25	Nonlinear optical ASnX (A = Na, H; X = N, P) nanosheets with divalent tin lone electron pair effect by first-principles design. Nanoscale, 2020, 12, 14895-14902.	2.8	10
26	Inorganic planar π -conjugated groups in nonlinear optical crystals: review and outlook. Inorganic Chemistry Frontiers, 2020, 7, 839-852.	3.0	93
27	$\text{Cs}_2\text{NaVCl}_6$: A Pb-Free Halide Double Perovskite with Strong Visible and Near-Infrared Light Absorption. ACS Applied Materials & Interfaces, 2019, 11, 38648-38653.	4.0	39
28	Poly(difluorophosphazene) as the First Deep-Ultraviolet Nonlinear Optical Polymer: A First-Principles Prediction. Angewandte Chemie - International Edition, 2019, 58, 10250-10254.	7.2	23
29	Poly(difluorophosphazene) as the First Deep-Ultraviolet Nonlinear Optical Polymer: A First-Principles Prediction. Angewandte Chemie, 2019, 131, 10356-10360.	1.6	11
30	Deep-ultraviolet nonlinear optical crystal $\text{NaBe}_2\text{BO}_3\text{F}_2$ Structure, growth and optical properties. Journal of Crystal Growth, 2019, 518, 45-50.	0.7	17
31	Lone-Pair Enhanced Birefringence in an Alkaline-Earth Metal Tin(II) Phosphate $\text{BaSn}_2(\text{PO}_4)_2$. Chemistry - A European Journal, 2019, 25, 5648-5651.	1.7	95
32	Prediction of MCO [M = S, (Cl ₂ B) ₃] Systems with Giant Optical Birefringence and Nonlinearity in the Deep-Ultraviolet Region. Inorganic Chemistry, 2019, 58, 77-80.	1.9	4
33	Recent advances and future perspectives on infrared nonlinear optical metal halides. Coordination Chemistry Reviews, 2019, 380, 83-102.	9.5	166
34	Significantly enhanced magnetoresistance in monolayer WTe_2 via heterojunction engineering: a first-principles study. Nanoscale, 2018, 10, 22231-22236.	2.8	11
35	Cyano-Based Materials with Giant Optical Anisotropy and Second Harmonic-Generation Effect. Inorganic Chemistry, 2018, 57, 15001-15008.	1.9	16
36	Two Novel Deep-Ultraviolet Nonlinear Optical Crystals with Shorter Phase-Matching Second Harmonic Generation than $\text{KBe}_2\text{BO}_3\text{F}_2$: A First-Principles Prediction (Phys. Status Solidi RRL 9/2018). Physica Status Solidi - Rapid Research Letters, 2018, 12, 1870330.	1.2	0

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37	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
38	Two Novel Deep-Ultraviolet Nonlinear Optical Crystals with Shorter Phase-Matching Second Harmonic Generation than KBe ₂ BO ₃ F ₂ : A First-Principles Prediction. <i>Physica Status Solidi - Rapid Research Letters</i> , 2018, 12, 1800276.	1.2	15
39	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 - International Edition</i> , 2018, 57, 8968-8972.	7.2	200
40	Removal of A-Site Alkali and Alkaline Earth Metal Cations in KBe ₂ BO ₃ F ₂ -Type Layered Structures To Enhance the Deep-Ultraviolet Nonlinear Optical Capability. <i>Inorganic Chemistry</i> , 2018, 57, 11146-11156.	1.9	37
41	Molecular Construction Using (C ₃ N ₃ O ₃) ³⁻ Anions: Analysis and Prospect for Inorganic Metal Cyanurates Nonlinear Optical Materials. <i>Crystal Growth and Design</i> , 2017, 17, 4015-4020.	1.4	114
42	Mid-Infrared Nonlinear Optical Materials Based on Metal Chalcogenides: Structure-Property Relationship. <i>Crystal Growth and Design</i> , 2017, 17, 2254-2289.	1.4	266
43	Ba _{1.31} Sr _{3.69} (BO ₃) ₃ Cl: A new structure type in the M ₅ (BO ₃) ₃ Cl (M = divalent cation) system. <i>Journal of Alloys and Compounds</i> , 2017, 699, 136-143.	2.8	11
44	Rational Design of Deep-Ultraviolet Nonlinear Optical Materials in Fluorooxoborates: Toward Optimal Planar Configuration. <i>Chemistry of Materials</i> , 2017, 29, 7098-7102.	3.2	136
45	Analysis and prediction of mid-IR nonlinear optical metal sulfides with diamond-like structures. <i>Coordination Chemistry Reviews</i> , 2017, 333, 57-70.	9.5	278
46	Reversible switching between pressure-induced amorphization and thermal-driven recrystallization in VO ₂ (B) nanosheets. <i>Nature Communications</i> , 2016, 7, 12214.	5.8	47
47	Na ₃ Y ₃ (BO ₃) ₄ : a new noncentrosymmetric borate with an open-framework structure. <i>Dalton Transactions</i> , 2016, 45, 7205-7208.	1.6	24
48	Calcium-decorated carbon nanostructures for the selective capture of carbon dioxide. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29086-29091.	1.3	15
49	Rb ₂ SeOCl ₄ ·H ₂ O: a polar material among the alkali metal selenite halides with a strong SHG response. <i>Dalton Transactions</i> , 2016, 45, 17723-17728.	1.6	15
50	Be ₂ BO ₃ F: A Phase of Beryllium Fluoride Borate Derived from KBe ₂ BO ₃ F ₂ with Short UV Absorption Edge. <i>Inorganic Chemistry</i> , 2016, 55, 6586-6591.	1.9	36
51	Ba ₃ FeS ₄ Br: A 0D Iron-Based Chalcogenide with Unusual Magnetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 1359-1363.	1.0	7
52	High pressure behaviour and elastic properties of a dense inorganic-organic framework. <i>Dalton Transactions</i> , 2016, 45, 4303-4308.	1.6	26
53	Midinfrared Nonlinear Optical Thiophosphates from LiZnPS ₄ to AgZnPS ₄ : A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2016, 55, 3724-3726.	1.9	78
54	RbIO ₃ and RbIO ₂ F ₂ : Two Promising Nonlinear Optical Materials in Mid-IR Region and Influence of Partially Replacing Oxygen with Fluorine for Improving Laser Damage Threshold. <i>Chemistry of Materials</i> , 2016, 28, 1413-1418.	3.2	107

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55	Designing a Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material without a Structural Instability Problem. <i>Journal of the American Chemical Society</i> , 2016, 138, 2961-2964.	6.6	220
56	Negative linear compressibility in a crystal of BiB_3O_6 . <i>Scientific Reports</i> , 2015, 5, 13432.	1.6	28
57	Isotropic Negative Area Compressibility over Large Pressure Range in Potassium Beryllium Fluoroborate and its Potential Applications in Deep Ultraviolet Region. <i>Advanced Materials</i> , 2015, 27, 4851-4857.	11.1	52
58	Nanostructured Ni_2P as a Robust Catalyst for the Hydrolytic Dehydrogenation of Ammonia-Borane. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 15725-15729.	7.2	204
59	Significantly Enhanced Infrared Emissivity of LaAlO_3 by Co^{2+} and Cr^{3+} Doping with Energy-Saving Applications. <i>Journal of the American Ceramic Society</i> , 2015, 98, 2336-2339.	1.9	38
60	An outstanding second-harmonic generation material $\text{BiB}_2\text{O}_4\text{F}$: exploiting the electron-withdrawing ability of fluorine. <i>Inorganic Chemistry Frontiers</i> , 2015, 2, 170-176.	3.0	82
61	$\text{K}_5\text{Mo}_4\text{O}_{14}\text{F}$: A Novel Fluorinated Polyoxomolybdate and Its Structural Stability. <i>Inorganic Chemistry</i> , 2015, 54, 6066-6068.	1.9	7
62	Syntheses, structures, and optical properties of $\text{Ba}_4\text{Ga}_4\text{SnSe}_{12}$ and $\text{Ba}_6\text{Ga}_2\text{SnSe}_{11}$. <i>Dalton Transactions</i> , 2015, 44, 2259-2266.	1.6	18
63	Sn_2SiS_4 , synthesis, structure, optical and electronic properties. <i>Optical Materials</i> , 2015, 47, 379-385.	1.7	14
64	PbGa_4S_7 : a wide-gap nonlinear optical material. <i>Journal of Materials Chemistry C</i> , 2015, 3, 3060-3067.	2.7	80
65	$\text{SnGa}_2\text{GeS}_6$: synthesis, structure, linear and nonlinear optical properties. <i>Dalton Transactions</i> , 2015, 44, 7404-7410.	1.6	40
66	Metal Thiophosphates with Good Mid-infrared Nonlinear Optical Performances: A First-Principles Prediction and Analysis. <i>Journal of the American Chemical Society</i> , 2015, 137, 13049-13059.	6.6	345
67	First-Principles Design of a Deep-Ultraviolet Nonlinear-Optical Crystal from $\text{KBe}_2\text{BO}_3\text{F}_2$ to $\text{NH}_4\text{Be}_2\text{BO}_3\text{F}_2$. <i>Inorganic Chemistry</i> , 2015, 54, 10533-10535.	1.9	85
68	First-Principles Evaluation of the Alkali and/or Alkaline Earth Beryllium Borates in Deep Ultraviolet Nonlinear Optical Applications. <i>ACS Photonics</i> , 2015, 2, 1183-1191.	3.2	117
69	Enhanced photocatalytic H_2 -evolution by immobilizing CdS nanocrystals on ultrathin $\text{Co}_{0.85}\text{Se}/\text{RGO}$ -PEI nanosheets. <i>Journal of Materials Chemistry A</i> , 2015, 3, 18711-18717.	5.2	51
70	Crystal structure and Raman spectrum of $\text{Ba}_2\text{Pb}(\text{B}_3\text{O}_6)_2$. <i>Materials Chemistry and Physics</i> , 2015, 163, 501-506.	2.0	6
71	The mechanism for the nonlinear optical properties in $\text{La}_9\text{Na}_3\text{B}_8\text{O}_{27}$, $\text{La}_2\text{Na}_3\text{B}_3\text{O}_9$ and $\text{La}_2\text{CaB}_{10}\text{O}_{19}$: <i>ab initio</i> studies. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 485501.	0.7	7
72	Synthesis of NiGa_2O_4 Octahedron Nanocrystal with Exposed {111} Facets and Enhanced Efficiency of Photocatalytic Water Splitting. <i>ChemPlusChem</i> , 2015, 80, 223-230.	1.3	18

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73	Structures and optical properties of two phases of SrMgF ₄ . Physical Chemistry Chemical Physics, 2015, 17, 500-508.	1.3	9
74	Development of nonlinear optical materials promoted by density functional theory simulations. International Journal of Modern Physics B, 2014, 28, 1430018.	1.0	27
75	A novel Bi-based phosphomolybdate photocatalyst K ₂ Bi(PO ₄)(MoO ₄): Crystal structure, electronic structure and photocatalytic activity. Materials Research Bulletin, 2014, 51, 455-459.	2.7	20
76	K ₃ MoPO ₇ : the first molybdenum phosphate with edge-sharing MoO ₆ octahedra and PO ₄ tetrahedra. RSC Advances, 2014, 4, 27122-27125.	1.7	8
77	First-principles materials applications and design of nonlinear optical crystals. Journal Physics D: Applied Physics, 2014, 47, 253001.	1.3	201
78	A promising new nonlinear optical crystal with high laser damage threshold for application in the IR region: synthesis, crystal structure and properties of noncentrosymmetric CsHgBr ₃ . Journal of Materials Chemistry C, 2014, 2, 6796-6801.	2.7	20
79	Syntheses, structures, optical properties, and electronic structures of KBaMSe ₃ (M = As, Sb). Journal of Alloys and Compounds, 2014, 617, 287-291.	2.8	19
80	Noncentrosymmetric chalcogenide NaBa ₄ Ge ₃ S ₁₀ Cl with large band gap and IR NLO response. Journal of Materials Chemistry C, 2014, 2, 4590-4596.	2.7	96
81	Three new chalcogenides, Ba ₄ Ge ₂ PbS ₈ Br ₂ , Ba ₄ Ge ₂ PbSe ₈ Br ₂ and Ba ₄ Ge ₂ SnS ₈ Br ₂ : Syntheses, crystal structures, band gaps, and electronic structures. Journal of Alloys and Compounds, 2014, 611, 422-426.	2.8	3
82	Prospects for Fluoride Carbonate Nonlinear Optical Crystals in the UV and Deep-UV Regions. Journal of Physical Chemistry C, 2013, 117, 25684-25692.	1.5	92
83	First principles selection and design of mid-IR nonlinear optical halide crystals. Journal of Materials Chemistry C, 2013, 1, 7363.	2.7	117
84	Ba ₆ Sn ₆ Se ₁₃ : a new mixed valence selenostannate with NLO property. Dalton Transactions, 2013, 42, 13635.	1.6	43
85	KS ₂ P ₃ : A new layered phosphidopolysilicate (IV). Journal of Solid State Chemistry, 2013, 205, 129-133.	1.4	18
86	Ln ₃ FeGaQ ₇ : A new series of transition-metal rare-earth chalcogenides. Journal of Solid State Chemistry, 2013, 202, 269-275.	1.4	23
87	K ₂ FeGe ₃ Se ₈ : A New Antiferromagnetic Iron Selenide. Inorganic Chemistry, 2013, 52, 2022-2028.	1.9	24
88	Structural, Spectroscopic, and Electronic Properties of Cubic G ₀ -Rb ₂ KTiOF ₅ Oxyfluoride. Journal of Physical Chemistry C, 2013, 117, 7269-7278.	1.5	38
89	Bandgaps in the deep ultraviolet borate crystals: Prediction and improvement. Applied Physics Letters, 2013, 102, 231904.	1.5	47
90	Hg ₂ Br ₃ : a new mixed halide nonlinear optical material in the infrared region. CrystEngComm, 2013, 15, 4196.	1.3	24

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91	Synthesis, Crystal Structure, Magnetic Property, and Electronic Structure of Ba ₂ YbInSe ₅ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1021-1025.	0.6	5
92	Two Novel Bi-Based Borate Photocatalysts: Crystal Structure, Electronic Structure, Photoelectrochemical Properties, and Photocatalytic Activity under Simulated Solar Light Irradiation. Journal of Physical Chemistry C, 2013, 117, 22986-22994.	1.5	334
93	Two novel nonlinear optical carbonates in the deep-ultraviolet region: KBeCO ₃ F and RbAlCO ₃ F ₂ . Scientific Reports, 2013, 3, 1366.	1.6	79
94	<i>Ab initio</i> studies on the optical effects in the deep ultraviolet nonlinear optical crystals of the KBe ₂ BO ₃ F ₂ family. Journal of Physics Condensed Matter, 2012, 24, 335503.	0.7	40
95	Strategy for the optical property studies in ultraviolet nonlinear optical crystals from density functional theory. Computational Materials Science, 2012, 60, 99-104.	1.4	71
96	Separable states and geometric phases of an interacting two-spin system. Physical Review A, 2010, 81, .	1.0	8
97	Experimental verification of isotropic and polarization properties of high permittivity-based metamaterial. Physical Review B, 2009, 80, .	1.1	29
98	Isotropic negative permeability composite based on Mie resonance of the BST-MgO dielectric medium. Science Bulletin, 2008, 53, 3272-3276.	4.3	9
99	Experimental demonstration of tunable negative phase velocity and negative refraction in a ferromagnetic/ferroelectric composite metamaterial. Applied Physics Letters, 2008, 93, .	1.5	23
100	Magnetically tunable negative permeability metamaterial composed by split ring resonators and ferrite rods. Optics Express, 2008, 16, 8825.	1.7	81
101	Ferrite-based magnetically tunable left-handed metamaterial composed of SRRs and wires. Optics Express, 2008, 16, 17269.	1.7	45
102	Magnetic control of negative permeability metamaterials based on liquid crystals. Applied Physics Letters, 2008, 92, .	1.5	67
103	Transparency cloak based on High-k BST rods. , 2008, , .		2
104	Magnetic tuning of electrically resonant metamaterial with inclusion of ferrite. Applied Physics Letters, 2008, 93, .	1.5	17
105	Tunable negative permeability in an isotropic dielectric composite. Applied Physics Letters, 2008, 92, .	1.5	78