Lei Kang

List of Publications by Year
in descending order

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105	5,801	76196	76769
papers	citations	40	74
		h-index	g-index

120	120	120	3189
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Metal Thiophosphates with Good Mid-infrared Nonlinear Optical Performances: A First-Principles Prediction and Analysis. Journal of the American Chemical Society, 2015, 137, 13049-13059.	6.6	345
2	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
3	Analysis and prediction of mid-IR nonlinear optical metal sulfides with diamond-like structures. Coordination Chemistry Reviews, 2017, 333, 57-70.	9.5	278
4	Mid-Infrared Nonlinear Optical Materials Based on Metal Chalcogenides: Structureâ€“Property Relationship. Crystal Growth and Design, 2017, 17, 2254-2289.	1.4	266
5	Designing a Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material without a Structural Instability Problem. Journal of the American Chemical Society, 2016, 138, 2961-2964.	6.6	220
6	Nanostructured Ni₂P as a Robust Catalyst for the Hydrolytic Dehydrogenation of Ammoniaâ€“Borane. Angewandte Chemie - International Edition, 2015, 54, 15725-15729.	7.2	204
7	First-principles materials applications and design of nonlinear optical crystals. Journal Physics D: Applied Physics, 2014, 47, 253001.	1.3	201
8	NH₄Be₂BO₃F₂ and Î³â€²-Be₂BO₃F: Overcoming the Layering Habit in KBe₂BO₃F₂ for the Nextâ€Generation Deepâ€Ultraviolet Nonlinear Optical Materials. Angewandte Chemie - International Edition, 2018, 57, 8968-8972.	7.2	200
9	First-Principles Design and Simulations Promote the Development of Nonlinear Optical Crystals. Accounts of Chemical Research, 2020, 53, 209-217.	7.6	194
10	Recent advances and future perspectives on infrared nonlinear optical metal halides. Coordination Chemistry Reviews, 2019, 380, 83-102.	9.5	166
11	Rational Design of Deep-Ultraviolet Nonlinear Optical Materials in Fluorooxoborates: Toward Optimal Planar Configuration. Chemistry of Materials, 2017, 29, 7098-7102.	3.2	136
12	First principles selection and design of mid-IR nonlinear optical halide crystals. Journal of Materials Chemistry C, 2013, 1, 7363.	2.7	117
13	First-Principles Evaluation of the Alkali and/or Alkaline Earth Beryllium Borates in Deep Ultraviolet Nonlinear Optical Applications. ACS Photonics, 2015, 2, 1183-1191.	3.2	117
14	Molecular Construction Using (C₃N₃O₃)^{3â€“} Anions: Analysis and Prospect for Inorganic Metal Cyanurates Nonlinear Optical Materials. Crystal Growth and Design, 2017, 17, 4015-4020.	1.4	114
15	RbIO₃ and RbIO₂F₂: Two Promising Nonlinear Optical Materials in Mid-IR Region and Influence of Partially Replacing Oxygen with Fluorine for Improving Laser Damage Threshold. Chemistry of Materials, 2016, 28, 1413-1418.	3.2	107
16	Noncentrosymmetric chalcohalide NaBa₄Ge₃S₁₀Cl with large band gap and IR NLO response. Journal of Materials Chemistry C, 2014, 2, 4590-4596.	2.7	96
17	Loneâ€Pair Enhanced Birefringence in an Alkalineâ€Earth Metal Tin(II) Phosphate BaSn₂(PO₄)₂. Chemistry - A European Journal, 2019, 25, 5648-5651.	1.7	95
18	Inorganic planar Ï€-conjugated groups in nonlinear optical crystals: review and outlook. Inorganic Chemistry Frontiers, 2020, 7, 839-852.	3.0	93

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19	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
20	LiZn(OH)CO₃: A Deepâ€Ultraviolet Nonlinear Optical Hydroxycarbonate Designed from a Diamondâ€like Structure. Angewandte Chemie - International Edition, 2021, 60, 13574-13578.	7.2	88
21	First-Principles Design of a Deep-Ultraviolet Nonlinear-Optical Crystal from KBe₂BO₃F₂ to NH₄Be₂BO₃F₂. Inorganic Chemistry, 2015, 54, 10533-10535.	1.9	85
22	An outstanding second-harmonic generation material BiB₂O₄F: exploiting the electron-withdrawing ability of fluorine. Inorganic Chemistry Frontiers, 2015, 2, 170-176.	3.0	82
23	Magnetically tunable negative permeability metamaterial composed by split ring resonators and ferrite rods. Optics Express, 2008, 16, 8825.	1.7	81
24	PbGa₄S₇: a wide-gap nonlinear optical material. Journal of Materials Chemistry C, 2015, 3, 3060-3067.	2.7	80
25	Two novel nonlinear optical carbonates in the deep-ultraviolet region: KBeCO3F and RbAlCO3F2. Scientific Reports, 2013, 3, 1366.	1.6	79
26	Tunable negative permeability in an isotropic dielectric composite. Applied Physics Letters, 2008, 92, .	1.5	78
27	Midinfrared Nonlinear Optical Thiophosphates from LiZnPS₄ to AgZnPS₄: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2016, 55, 3724-3726.	1.9	78
28	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
29	Magnetic control of negative permeability metamaterials based on liquid crystals. Applied Physics Letters, 2008, 92, .	1.5	67
30	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
31	NH₄Be₂BO₃F₂ and Î³â€Be₂BO₃F: Overcoming the Layering Habit in KBe₂BO₃F₂ for the Nextâ€Generation Deepâ€Ultraviolet Nonlinear Optical Materials. Angewandte Chemie, 2018, 130, 9106-9110.	1.6	63
32	Deep-ultraviolet nonlinear optical crystals: concept development and materials discovery. Light: Science and Applications, 2022, 11, .	7.7	55
33	Isotropic Negative Area Compressibility over Large Pressure Range in Potassium Beryllium Fluoroborate and its Potential Applications in Deep Ultraviolet Region. Advanced Materials, 2015, 27, 4851-4857.	11.1	52
34	Enhanced photocatalytic H₂-evolution by immobilizing CdS nanocrystals on ultrathin Co_{0.85}Se/RGOâ€“PEI nanosheets. Journal of Materials Chemistry A, 2015, 3, 18711-18717.	5.2	51
35	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
36	Bandgaps in the deep ultraviolet borate crystals: Prediction and improvement. Applied Physics Letters, 2013, 102, 231904.	1.5	47

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37	Reversible switching between pressure-induced amorphization and thermal-driven recrystallization in VO2(B) nanosheets. Nature Communications, 2016, 7, 12214.	5.8	47
38	Ferrite-based magnetically tunable left-handed metamaterial composed of SRRs and wires. Optics Express, 2008, 16, 17269.	1.7	45
39	Ba6Sn6Se13: a new mixed valence selenostannate with NLO property. Dalton Transactions, 2013, 42, 13635.	1.6	43
40	Ab initiostudies on the optical effects in the deep ultraviolet nonlinear optical crystals of the KBe₂BO₃F₂family. Journal of Physics Condensed Matter, 2012, 24, 335503.	0.7	40
41	SnGa₂GeS₆: synthesis, structure, linear and nonlinear optical properties. Dalton Transactions, 2015, 44, 7404-7410.	1.6	40
42	Cs₂NaVCl₆: 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
43	Structural, Spectroscopic, and Electronic Properties of Cubic G0-Rb₂KTiOF₅ Oxyfluoride. Journal of Physical Chemistry C, 2013, 117, 7269-7278.	1.5	38
44	Significantly Enhanced Infrared Emissivity of LaAlO₃ by Coâ€Doping with Ca²⁺ and Cr³⁺ for Energyâ€Saving Applications. Journal of the American Ceramic Society, 2015, 98, 2336-2339.	1.9	38
45	Removal of A-Site Alkali and Alkaline Earth Metal Cations in KBe₂BO₃F₂-Type Layered Structures To Enhance the Deep-Ultraviolet Nonlinear Optical Capability. Inorganic Chemistry, 2018, 57, 11146-11156.	1.9	37
46	Be₂BO₃F: A Phase of Beryllium Fluoride Borate Derived from KBe₂BO₃F₂ with Short UV Absorption Edge. Inorganic Chemistry, 2016, 55, 6586-6591.	1.9	36
47	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
48	Experimental verification of isotropic and polarization properties of high permittivity-based metamaterial. Physical Review B, 2009, 80, .	1.1	29
49	Negative linear compressibility in a crystal of Î±-BiB3O6. Scientific Reports, 2015, 5, 13432.	1.6	28
50	Development of nonlinear optical materials promoted by density functional theory simulations. International Journal of Modern Physics B, 2014, 28, 1430018.	1.0	27
51	High pressure behaviour and elastic properties of a dense inorganicâ€“organic framework. Dalton Transactions, 2016, 45, 4303-4308.	1.6	26
52	Layered oxide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>9</mml:mn></mml:msub></mml:mrow></mml:math> with a deep-ultraviolet band gap and a strong and robust second-harmonic generation. Physical Review B, 2	1.1	25
53	K2FeGe3Se8: A New Antiferromagnetic Iron Selenide. Inorganic Chemistry, 2013, 52, 2022-2028.	1.9	24
54	Hg2Br3I: a new mixed halide nonlinear optical material in the infrared region. CrystEngComm, 2013, 15, 4196.	1.3	24

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55	Na₃Y₃(BO₃)₄: a new noncentrosymmetric borate with an open-framework structure. Dalton Transactions, 2016, 45, 7205-7208.	1.6	24
56	Experimental demonstration of tunable negative phase velocity and negative refraction in a ferromagnetic/ferroelectric composite metamaterial. Applied Physics Letters, 2008, 93, .	1.5	23
57	Ln3FeGaQ7: A new series of transition-metal rare-earth chalcogenides. Journal of Solid State Chemistry, 2013, 202, 269-275.	1.4	23
58	Poly(difluorophosphazene) as the First Deepâ€Ultraviolet Nonlinear Optical Polymer: A Firstâ€Principles Prediction. Angewandte Chemie - International Edition, 2019, 58, 10250-10254.	7.2	23
59	A novel Bi-based phosphomolybdate photocatalyst K2Bi(PO4)(MoO4): Crystal structure, electronic structure and photocatalytic activity. Materials Research Bulletin, 2014, 51, 455-459.	2.7	20
60	A promising new nonlinear optical crystal with high laser damage threshold for application in the IR region: synthesis, crystal structure and properties of noncentrosymmetric CsHgBr₃. Journal of Materials Chemistry C, 2014, 2, 6796-6801.	2.7	20
61	Second harmonic generation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi>Si</mml:mi><mml:mn mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> -type layers. Physical Review B, 2021, 103, .	1.1	20
62	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
63	Anomalous mechanical materials squeezing three-dimensional volume compressibility into one dimension. Nature Communications, 2020, 11, 5593.	5.8	19
64	KSi2P3: A new layered phosphidopolysilicate (IV). Journal of Solid State Chemistry, 2013, 205, 129-133.	1.4	18
65	Syntheses, structures, and optical properties of Ba₄Ga₄SnSe₁₂and Ba₆Ga₂SnSe₁₁. Dalton Transactions, 2015, 44, 2259-2266.	1.6	18
66	Synthesis of NiGa2O4Octahedron Nanocrystal with Exposed {111} Facets and Enhanced Efficiency of Photocatalytic Water Splitting. ChemPlusChem, 2015, 80, 223-230.	1.3	18
67	Electrochemical ammonia synthesis from nitrite assisted by in situ generated hydrogen atoms on a nickel phosphide catalyst. Chemical Communications, 2021, 57, 7176-7179.	2.2	18
68	Magnetic tuning of electrically resonant metamaterial with inclusion of ferrite. Applied Physics Letters, 2008, 93, .	1.5	17
69	Deep-ultraviolet nonlinear optical crystal NaBe2BO3F2â€”Structure, growth and optical properties. Journal of Crystal Growth, 2019, 518, 45-50.	0.7	17
70	Deepâ€Ultraviolet Nonlinearâ€Optical vanâ€derâ€Waals Beryllium Borates**. Angewandte Chemie - International Edition, 2021, 60, 16680-16686.	7.2	17
71	Cyano-Based Materials with Giant Optical Anisotropy and Second Harmonic-Generation Effect. Inorganic Chemistry, 2018, 57, 15001-15008.	1.9	16
72	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

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73	Calcium-decorated carbon nanostructures for the selective capture of carbon dioxide. Physical Chemistry Chemical Physics, 2016, 18, 29086-29091.	1.3	15
74	Rb2SeOCl4Â·H2O: a polar material among the alkali metal selenite halides with a strong SHG response. Dalton Transactions, 2016, 45, 17723-17728.	1.6	15
75	Two Novel Deepâ€Ultraviolet Nonlinear Optical Crystals with Shorter Phaseâ€Matching Second Harmonic Generation than KBe₂BO₃F₂: A Firstâ€Principles Prediction. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800276.	1.2	15
76	Sn2SiS4, synthesis, structure, optical and electronic properties. Optical Materials, 2015, 47, 379-385.	1.7	14
77	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
78	Ba 1.31 Sr 3.69 (BO 3) 3 Cl: A new structure type in the M 5 (BO 3) 3 Cl (MÂ=Âbivalent cation) system. Journal of Alloys and Compounds, 2017, 699, 136-143.	2.8	11
79	Significantly enhanced magnetoresistance in monolayer WTe2via heterojunction engineering: a first-principles study. Nanoscale, 2018, 10, 22231-22236.	2.8	11
80	Poly(difluorophosphazene) as the First Deepâ€Ultraviolet Nonlinear Optical Polymer: A Firstâ€Principles Prediction. Angewandte Chemie, 2019, 131, 10356-10360.	1.6	11
81	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
82	Isotropic negative permeability composite based on Mie resonance of the BST-MgO dielectric medium. Science Bulletin, 2008, 53, 3272-3276.	4.3	9
83	Structures and optical properties of two phases of SrMgF₄. Physical Chemistry Chemical Physics, 2015, 17, 500-508.	1.3	9
84	LiZn(OH)CO 3 : A Deepâ€Ultraviolet Nonlinear Optical Hydroxycarbonate Designed from a Diamondâ€like Structure. Angewandte Chemie, 2021, 133, 13686-13690.	1.6	9
85	Role of interlayer coupling in second harmonic generation in bilayer transition metal dichalcogenides. Physical Review B, 2022, 105, .	1.1	9
86	Mid-Infrared Nonlinear Optical Halides with Diamond-like Structures: A Theoretical and Experimental Study. Chemistry of Materials, 2022, 34, 5301-5310.	3.2	9
87	Separable states and geometric phases of an interacting two-spin system. Physical Review A, 2010, 81, .	1.0	8
88	K₃MoPO₇: the first molybdenum phosphate with edge-sharing MoO₆octahedra and PO₄tetrahedra. RSC Advances, 2014, 4, 27122-27125.	1.7	8
89	K5Mo4O14F: A Novel Fluorinated Polyoxomolybdate and Its Structural Stability. Inorganic Chemistry, 2015, 54, 6066-6068.	1.9	7
90	The mechanism for the nonlinear optical properties in La₉Na₃B₈O₂₇, La₂Na₃B₃O₉and La₂CaB₁₀O₁₉:ab initiostudies. Journal of Physics Condensed Matter, 2015, 27, 485501.	0.7	7

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91	Ba₃FeS₄Br: A 0D Ironâ€Based Chalcohalide with Unusual Magnetic Properties. European Journal of Inorganic Chemistry, 2016, 2016, 1359-1363.	1.0	7
92	Crystal structure and Raman spectrum of Ba2Pb(B3O6)2. Materials Chemistry and Physics, 2015, 163, 501-506.	2.0	6
93	Synthesis, Crystal Structure, Magnetic Property, and Electronic Structure of Ba₂YbInSe₅. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1021-1025.	0.6	5
94	Alloy Engineering of a Polar (Si,Ge)₂N₂O System for Controllable Second Harmonic Performance. Inorganic Chemistry, 2021, 60, 7381-7388.	1.9	5
95	Two metal-free cyanurate crystals with a large optical birefringence resulting from the combination of Ï€-conjugated units. Dalton Transactions, 2021, 50, 17495-17498.	1.6	5
96	Sliding Modulation in Nonlinear Optical Effect in Two-Dimensional van der Waals Cu₂MoS₄. ACS Applied Materials & Interfaces, 2022, 14, 9535-9543.	4.0	5
97	Prediction of MCO [M = S, (Cl₂B)₃B] Systems with Giant Optical Birefringence and Nonlinearity in the Deep-Ultraviolet Region. Inorganic Chemistry, 2019, 58, 77-80.	1.9	4
98	Deepâ€Ultraviolet Nonlinearâ€Optical vanâ€derâ€Waals Beryllium Borates**. Angewandte Chemie, 2021, 133, 16816-16822.	1.6	4
99	Fluorine Effects for Tunable Câ€“C and Câ€“S Bond Cleavage in Fluoro-Juliaâ€“Kocienski Intermediates. CCS Chemistry, 2021, 3, 1678-1689.	4.6	4
100	Three new chalcohalides, Ba4Ge2PbS8Br2, Ba4Ge2PbSe8Br2 and Ba4Ge2SnS8Br2: Syntheses, crystal structures, band gaps, and electronic structures. Journal of Alloys and Compounds, 2014, 611, 422-426.	2.8	3
101	Transparency cloak based on High-k BST rods. , 2008, , .		2
102	Tourmaline with ultraviolet optical nonlinearity: Emergent material discovery from mineral. Journal of Alloys and Compounds, 2022, 892, 162235.	2.8	2
103	Surface functionalization of phosphorene via P-H bond for ambient protection and robust photocatalytic H2 evolution. Science China Materials, 2022, 65, 1245-1251.	3.5	2
104	Novel van der Waals Deepâ€UV Nonlinear Optical Materials. Chemistry - A European Journal, 2021, 27, 17269-17272.	1.7	1
105	Two Novel Deep-Ultraviolet Nonlinear Optical Crystals with Shorter Phase-Matching Second Harmonic Generation than KBe2 BO3 F2 : A First-Principles Prediction (Phys. Status Solidi RRL 9/2018). Physica Status Solidi - Rapid Research Letters, 2018, 12, 1870330.	1.2	0