Emmanouil Kioupakis

List of Publications by Year
in descending order

97	4,901	101384 36	98622 67
papers	citations	h-index	g-index

101	101	101	7211
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. Applied Physics Letters, 2011, 98, .	1.5	447
2	Anisotropic Spin Transport and Strong Visible-Light Absorbance in Few-Layer SnSe and GeSe. Nano Letters, 2015, 15, 6926-6931.	4.5	290
3	Electrochemical Window of the Li-Ion Solid Electrolyte Li₇La₃Zr₂O₁₂. ACS Energy Letters, 2017, 2, 462-468.	8.8	255
4	Phase Stability and Transport Mechanisms in Antiperovskite Li₃OCl and Li₃OBr Superionic Conductors. Chemistry of Materials, 2013, 25, 4663-4670.	3.2	204
5	Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes. Applied Physics Letters, 2012, 101, .	1.5	165
6	Electronic and Optical Properties of Two-Dimensional GaN from First-Principles. Nano Letters, 2017, 17, 7345-7349.	4.5	160
7	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	2.9	157
8	Phonon-Assisted Optical Absorption in Silicon from First Principles. Physical Review Letters, 2012, 108, 167402.	2.9	143
9	Tuning Ionic Transport in Memristive Devices by Graphene with Engineered Nanopores. ACS Nano, 2016, 10, 3571-3579.	7.3	139
10	Quasiparticle band structures and thermoelectric transport properties of p-type SnSe. Journal of Applied Physics, 2015, 117, .	1.1	135
11	Quasiparticle effects in the bulk and surface-state bands of Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	118
12	Free-carrier absorption in nitrides from first principles. Physical Review B, 2010, 81, .	1.1	109
13	Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices. New Journal of Physics, 2013, 15, 125006.	1.2	109
14	Fundamental limits on optical transparency of transparent conducting oxides: Free-carrier absorption in SnO2. Applied Physics Letters, 2012, 100, .	1.5	93
15	Spatially resolved electronic and vibronic properties of single diamondoid molecules. Nature Materials, 2008, 7, 38-42.	13.3	87
16	Charge Transition of Oxygen Vacancies during Resistive Switching in Oxide-Based RRAM. ACS Applied Materials & Interfaces, 2019, 11, 11579-11586.	4.0	82
17	First-principles calculations of indirect Auger recombination in nitride semiconductors. Physical Review B, 2015, 92, .	1.1	77
18	Deep ultraviolet emission from ultra-thin GaN/AlN heterostructures. Applied Physics Letters, 2016, 109, .	1.5	73

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19	Determination of Internal Loss in Nitride Lasers from First Principles. Applied Physics Express, 2010, 3, 082101.	1.1	64
20	Protecting the properties of monolayer MoS2 on silicon based substrates with an atomically thin buffer. Scientific Reports, 2016, 6, 20890.	1.6	64
21	Unexpectedly Strong Auger Recombination in Halide Perovskites. Advanced Energy Materials, 2018, 8, 1801027.	10.2	64
22	First-principles calculations of the near-edge optical properties of Î²-Ga2O3. Applied Physics Letters, 2016, 109, 212104.	1.5	62
23	Impact of carrier localization on recombination in InGaN quantum wells and the efficiency of nitride light-emitting diodes: Insights from theory and numerical simulations. Applied Physics Letters, 2017, 111, .	1.5	62
24	Frenkel-like Wannier-Mott excitons in few-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pb</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2015, 91, .	1.1	61
25	Pb₇Bi₄Se₁₃: A Lillianite Homologue with Promising Thermoelectric Properties. Inorganic Chemistry, 2015, 54, 746-755.	1.9	60
26	Quasiparticle electronic structure of bismuth telluride in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>approximation. Physical Review B, 2010, 82, .	1.1	59
27	Predicting and Designing Optical Properties of Inorganic Materials. Annual Review of Materials Research, 2015, 45, 491-518.	4.3	56
28	Low-temperature structural and transport anomalies in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Se</mml:mi></mml:math>. Physical Review B, 2014, 89, .	1.1	54
29	Giant Ferroelectric Polarization in Ultrathin Ferroelectrics via Boundaryâ€Condition Engineering. Advanced Materials, 2017, 29, 1701475.	11.1	47
30	Band structure and carrier effective masses of boron arsenide: Effects of quasiparticle and spin-orbit coupling corrections. Applied Physics Letters, 2019, 114, .	1.5	46
31	Electronic and optical properties of oxygen vacancies in amorphous Ta₂O₅from first principles. Nanoscale, 2017, 9, 1120-1127.	2.8	45
32	Electronic and Optical Properties of Nanoporous Silicon for Solar-Cell Applications. ACS Photonics, 2015, 2, 208-215.	3.2	43
33	Vibrational and electron-phonon coupling properties of Î²-Ga2O3 from first-principles calculations: Impact on the mobility and breakdown field. AIP Advances, 2019, 9, .	0.6	40
34	Monolayer GaN excitonic deep ultraviolet light emitting diodes. Applied Physics Letters, 2020, 116, .	1.5	39
35	Stabilization of orthorhombic phase in single-crystal ZnSnN2 films. AIP Advances, 2016, 6, .	0.6	38
36	Impact of the stacking sequence on the bandgap and luminescence properties of bulk, bilayer, and monolayer hexagonal boron nitride. APL Materials, 2019, 7, .	2.2	38

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37	Alloy-Free Band Gap Tuning across the Visible Spectrum. Physical Review Letters, 2019, 122, 256403.	2.9	37
38	Rutile GeO2: An ultrawide-band-gap semiconductor with ambipolar doping. Applied Physics Letters, 2019, 114, .	1.5	37
39	Deep Ultraviolet Luminescence Due to Extreme Confinement in Monolayer GaN/Al(Ga)N Nanowire and Planar Heterostructures. Nano Letters, 2019, 19, 7852-7858.	4.5	35
40	Semiconducting High-Entropy Chalcogenide Alloys with Ambi-ionic Entropy Stabilization and Ambipolar Doping. Chemistry of Materials, 2020, 32, 6070-6077.	3.2	35
41	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>quasiparticle corrections to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:mo>â^•</mml:mo><mml:mi	1.1	34
42	Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2015, 92, .	1.1	34
43	Point defects and dopants of boron arsenide from first-principles calculations: Donor compensation and doping asymmetry. Applied Physics Letters, 2018, 113, .	1.5	33
44	Visible-Wavelength Polarized-Light Emission with Small-Diameter InN Nanowires. Nano Letters, 2014, 14, 3709-3714.	4.5	32
45	Theoretical limits of thermoelectric figure of merit inn-typeTiO2polymorphs. Physical Review B, 2015, 91, .	1.1	32
46	Electronic properties of tantalum pentoxide polymorphs from first-principles calculations. Applied Physics Letters, 2014, 105, 202108.	1.5	30
47	Auger Recombination in GaAs from First Principles. ACS Photonics, 2014, 1, 643-646.	3.2	30
48	Polarization-Dependent Raman Spectroscopy of Epitaxial TiO₂(B) Thin Films. Chemistry of Materials, 2015, 27, 7896-7902.	3.2	29
49	Room-temperature stability of excitons and transverse-electric polarized deep-ultraviolet luminescence in atomically thin GaN quantum wells. Applied Physics Letters, 2019, 115, .	1.5	29
50	Optical properties of cubic boron arsenide. Applied Physics Letters, 2020, 116, .	1.5	29
51	Magnetic frustration control through tunable stereochemically driven disorder in entropy-stabilized oxides. Physical Review Materials, 2019, 3, .	0.9	29
52	Boron arsenide heterostructures: lattice-matched heterointerfaces and strain effects on band alignments and mobility. Npj Computational Materials, 2020, 6, .	3.5	28
53	BInGaN alloys nearly lattice-matched to GaN for high-power high-efficiency visible LEDs. Applied Physics Letters, 2017, 111, .	1.5	26
54	III-nitride nanostructures: Emerging applications for Micro-LEDs, ultraviolet photonics, quantum optoelectronics, and artificial photosynthesis. Progress in Quantum Electronics, 2022, 85, 100401.	3.5	26

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55	Quasiparticle band structure and optical properties of rutile GeO2, an ultra-wide-band-gap semiconductor. Journal of Applied Physics, 2019, 126, .	1.1	23
56	Toward the predictive discovery of ambipolarly dopable ultra-wide-band-gap semiconductors: The case of rutile GeO2. Applied Physics Letters, 2021, 118, .	1.5	23
57	Effect of growth temperature on the structural and optical properties of few-layer hexagonal boron nitride by molecular beam epitaxy. Optics Express, 2018, 26, 23031.	1.7	22
58	Electron and hole mobility of rutile GeO2 from first principles: An ultrawide-bandgap semiconductor for power electronics. Applied Physics Letters, 2020, 117, .	1.5	22
59	Oxygen defect dominated photoluminescence emission of ScxAl1â^'xN grown by molecular beam epitaxy. Applied Physics Letters, 2021, 118, .	1.5	22
60	Memristors Based on (Zr, Hf, Nb, Ta, Mo, W) Highâ€Entropy Oxides. Advanced Electronic Materials, 2021, 7, 2001258.	2.6	22
61	Scalable Synthesis of Monolayer Hexagonal Boron Nitride on Graphene with Giant Bandgap Renormalization. Advanced Materials, 2022, 34, e2201387.	11.1	22
62	Enhanced doping efficiency of ultrawide band gap semiconductors by metal-semiconductor junction assisted epitaxy. Physical Review Materials, 2019, 3, .	0.9	21
63	First-principles study of high-field-related electronic behavior of group-III nitrides. Physical Review B, 2014, 90, .	1.1	20
64	Sustainable p-type copper selenide solar material with ultra-large absorption coefficient. Chemical Science, 2018, 9, 5405-5414.	3.7	20
65	Insights on the Synthesis, Crystal and Electronic Structures, and Optical and Thermoelectric Properties of Sr_{1â€“x}Sb_xHfSe₃ Orthorhombic Perovskite. Inorganic Chemistry, 2018, 57, 7402-7411.	1.9	20
66	Radiative and Auger recombination processes in indium nitride. Applied Physics Letters, 2018, 112, .	1.5	20
67	Controlling Defect Formation of Nanoscale AlN: Toward Efficient Current Conduction of Ultrawideâ€Bandgap Semiconductors. Advanced Electronic Materials, 2020, 6, 2000337.	2.6	19
68	Thermal conductivity of rutile germanium dioxide. Applied Physics Letters, 2020, 117, 102106.	1.5	19
69	Epitaxial stabilization of rutile germanium oxide thin film by molecular beam epitaxy. Applied Physics Letters, 2020, 117, .	1.5	19
70	Relativistic quasiparticle band structures of Mg2Si, Mg2Ge, and Mg2Sn: Consistent parameterization and prediction of Seebeck coefficients. Journal of Applied Physics, 2018, 123, .	1.1	18
71	Electronic and Optical Properties of Two-Dimensional Î±-PbO from First Principles. Chemistry of Materials, 2018, 30, 7124-7129.	3.2	17
72	High electron mobility of AlxGa1â^'xN evaluated by unfolding the DFT band structure. Applied Physics Letters, 2020, 117, 242105.	1.5	17

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73	Limitations of In2O3 as a transparent conducting oxide. Applied Physics Letters, 2019, 115, .	1.5	14
74	Engineering new limits to magnetostriction through metastability in iron-gallium alloys. Nature Communications, 2021, 12, 2757.	5.8	14
75	Phonon- and defect-limited electron and hole mobility of diamond and cubic boron nitride: A critical comparison. Applied Physics Letters, 2021, 119, .	1.5	14
76	Atomistic analysis of radiative recombination rate, Stokes shift, and density of states in c-plane InGaN/GaN quantum wells. Applied Physics Letters, 2020, 116, .	1.5	13
77	Designing interchain and intrachain properties of conjugated polymers for latent optical information encoding. Chemical Science, 2015, 6, 6980-6985.	3.7	12
78	Dielectric Engineering for Manipulating Exciton Transport in Semiconductor Monolayers. Nano Letters, 2021, 21, 8409-8417.	4.5	12
79	Atomistic analysis of Auger recombination in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>c</mml:mi></mml:math> -plane (In,Ga)N/GaN quantum wells: Temperature-dependent competition between radiative and nonradiative recombination. Physical Review B, 2022, 105, .	1.1	12
80	Auger recombination in sodium-iodide scintillators from first principles. Applied Physics Letters, 2015, 106, .	1.5	11
81	Surface phonons in the topological insulators Bi2Se3 and Bi2Te3. Solid State Communications, 2018, 271, 1-5.	0.9	10
82	BAlGaN alloys nearly lattice-matched to AlN for efficient UV LEDs. Applied Physics Letters, 2019, 115, .	1.5	10
83	Effect of strain on band alignment of GaAsSb/GaAs quantum wells. Journal of Applied Physics, 2017, 122, 045703.	1.1	8
84	Theoretical characterization and computational discovery of ultra-wide-band-gap semiconductors with predictive atomistic calculations. Journal of Materials Research, 2021, 36, 4616-4637.	1.2	7
85	Effects of local compositional and structural disorder on vacancy formation in entropy-stabilized oxides from first-principles. Npj Computational Materials, 2022, 8, .	3.5	7
86	Predictive Simulations for Tuning Electronic and Optical Properties of SubPc Derivatives. Journal of Electronic Materials, 2019, 48, 2962-2970.	1.0	5
87	Experimental and theoretical study of hole scattering in RF sputtered p-type Cu2O thin films. Applied Physics Letters, 2022, 120, .	1.5	5
88	Lattice-constant and band-gap tuning in wurtzite and zincblende BInGaN alloys. Journal of Applied Physics, 2019, 126, 055702.	1.1	4
89	Hyperspectral absorption of semiconductor monolayer crystals. Applied Physics Letters, 2020, 116, .	1.5	4
90	Cation-size mismatch as a predictive descriptor for structural distortion, configurational disorder, and valence-band splitting in II-IV-N2 semiconductors. Applied Physics Letters, 2021, 119, .	1.5	4

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91	Nanoscale AlGaN and BN: Molecular beam epitaxy, properties, and device applications. Semiconductors and Semimetals, 2021, , 153-189.	0.4	3
92	Impact of phonons and spin-orbit coupling on Auger recombination in InAs. Physical Review B, 2019, 100, .	1.1	2
93	Semiconducting character of LaN: Magnitude of the bandgap and origin of the electrical conductivity. AIP Advances, 2021, 11, .	0.6	2
94	Effect of Stacking Orientation on the Electronic and Optical Properties of Polar 2D III-Nitride Bilayers. Journal of Physical Chemistry C, 2021, 125, 16837-16842.	1.5	2
95	Publisher's Note: Low-temperature structural and transport anomalies inCu2Se[Phys. Rev. B89, 195209 (2014)]. Physical Review B, 2014, 89, .	1.1	1
96	Auger recombination in InAs: Role of spin-orbit coupling and phonons. , 2016, , .		1
97	Auger recombination in light-emitting materials. , 2014, , .		0