

# Liverios Lymerakis

## List of Publications by Year in descending order

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52

papers

1,873

citations

304743

22

h-index

254184

43

g-index

54

all docs

54

docs citations

54

times ranked

2706

citing authors

#	ARTICLE	IF	CITATIONS
1	Revealing the Design Principles of High-Performance Biological Composites Using Ab initio and Multiscale Simulations: The Example of Lobster Cuticle. <i>Advanced Materials</i> , 2010, 22, 519-526.	21.0	285
2	Large anisotropic adatom kinetics on nonpolar GaN surfaces: Consequences for surface morphologies and nanowire growth. <i>Physical Review B</i> , 2009, 79, .	3.2	172
3	Hydrogen-enhanced local plasticity at dilute bulk H concentrations: The role of H-H interactions and the formation of local hydrides. <i>Acta Materialia</i> , 2011, 59, 2969-2980.	7.9	132
4	Gallium adsorption on (0001) GaN surfaces. <i>Physical Review B</i> , 2003, 67, .	3.2	131
5	Strain Induced Deep Electronic States around Threading Dislocations in GaN. <i>Physical Review Letters</i> , 2004, 93, 196401.	7.8	107
6	Polarity in GaN and ZnO: Theory, measurement, growth, and devices. <i>Applied Physics Reviews</i> , 2016, 3, .	11.3	105
7	Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2011, 4, 129-145.	3.1	91
8	Blocking Growth by an Electrically Active Subsurface Layer: The Effect of Si as an Antisurfactant in the Growth of GaN. <i>Physical Review Letters</i> , 2013, 110, 036103.	7.8	66
9	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. <i>Physical Review Letters</i> , 2018, 121, 015702.	7.8	65
10	Chemically ordered Al <sub>x</sub> Ga <sub>1-x</sub> N alloys: Spontaneous formation of natural quantum wells. <i>Physical Review B</i> , 2005, 71, .	3.2	53
11	Understanding and controlling indium incorporation and surface segregation on InGaN surfaces: An ab initio approach. <i>Physical Review B</i> , 2014, 89, .	3.2	47
12	Hidden surface states at non-polar GaN (101̄A) facets: Intrinsic pinning of nanowires. <i>Applied Physics Letters</i> , 2013, 103, .	3.3	45
13	Ab initio study of thermodynamic, structural, and elastic properties of Mg-substituted crystalline calcite. <i>Acta Biomaterialia</i> , 2010, 6, 4506-4512.	8.3	44
14	A modified empirical potential for energetic calculations of planar defects in GaN. <i>Computational Materials Science</i> , 2003, 27, 43-49.	3.0	42
15	GaN(0001) surface states: Experimental and theoretical fingerprints to identify surface reconstructions. <i>Physical Review B</i> , 2013, 88, .	3.2	37
16	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. <i>Physical Review Materials</i> , 2018, 2, .	2.4	36
17	Morphology and surface reconstructions of GaN(11̄,00) surfaces. <i>Applied Physics Letters</i> , 2003, 82, 1793-1795.	3.3	35
18	Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2013, 20, 296-304.	3.1	32

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19	Selective-area growth of GaN nanowires on SiO <sub>2</sub> -masked Si (111) substrates by molecular beam epitaxy. Journal of Applied Physics, 2016, 119, 224305.	2.5	29
20	Band offsets at zincblende-wurtzite GaAs nanowire sidewall surfaces. Applied Physics Letters, 2013, 103, .	3.3	28
21	< i>Ab Initio</i> Based conformational study of the crystalline chitin. Biopolymers, 2013, 99, 22-34.	2.4	27
22	Effect of edge threading dislocations on the electronic structure of InN. Applied Physics Letters, 2011, 98, .	3.3	23
23	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. European Physical Journal Plus, 2011, 126, 1.	2.6	22
24	Polar AlN/GaN interfaces: Structures and energetics. Physica Status Solidi (A) Applications and Materials Science, 2009, 206, 1892-1897.	1.8	20
25	In situ scanning tunneling microscopy study of selective dissolution of Au <sub>3</sub> Cu and Cu <sub>3</sub> Au (001). Electrochimica Acta, 2011, 56, 1694-1700.	5.2	19
26	Origin of the unusually strong luminescence of <math>\text{Ga}_\text{N}</math>-type screw dislocations in GaN. Physical Review B, 2014, 90, .	3.2	19
27	Electronic structure of 1/6(202̄3) partial dislocations in wurtzite GaN. Journal of Applied Physics, 2011, 109, .	2.5	16
28	< i>Ab initio</i> based bulk and surface thermodynamics of InGaN alloys: Investigating the effects of strain and surface polarity. Physica Status Solidi (B): Basic Research, 2015, 252, 855-865.	1.5	16
29	Adsorption and desorption of hydrogen at nonpolar surfaces: Kinetics and impact on surface vibrational and electronic properties. Physical Review B, 2017, 95, .	3.2	15
30	Mechanism leading to semi-insulating property of carbon-doped GaN: Analysis of donor acceptor ratio and method for its determination. Journal of Applied Physics, 2021, 130, .	2.5	11
31	Separating strain from composition in unit cell parameter maps obtained from aberration corrected high resolution transmission electron microscopy imaging. Journal of Applied Physics, 2014, 115, 033113.	2.5	10
32	Ab-initio study of boron incorporation and compositional limits at GaN and AlN (0001) surfaces. AIP Advances, 2018, 8, .	1.3	10
33	Atomistic calculations on interfaces: Bridging the length and time scales. European Physical Journal: Special Topics, 2009, 177, 41-57.	2.6	9
34	Influence of strain on the indium incorporation in (0001) GaN. Physical Review Materials, 2020, 4, .	2.4	9
35	Substitutional synthesis of sub-nanometer InGaN/GaN quantum wells with high indium content. Scientific Reports, 2021, 11, 20606.	3.3	9
36	Atomic-scale models of interactions between inversion domain boundaries and intrinsic basal stacking faults in GaN. Diamond and Related Materials, 2002, 11, 905-909.	3.9	8

#	ARTICLE	IF	CITATIONS
37	Development of semipolar (11-22) LEDs on GaN templates. Proceedings of SPIE, 2016, , .	0.8	8
38	Reconstructions and electronic structure of (112 $\bar{A}$ -2) and (112 $\bar{A}$ -2 $\bar{A}$ ) semipolar AlN surfaces. Journal of Applied Physics, 2012, 112, 033510.	2.5	7
39	Role of hole confinement in the recombination properties of InGaN quantum structures. Scientific Reports, 2019, 9, 9047.	3.3	6
40	Fermi-level pinning and intrinsic surface states of Al $1\hat{x}$ In $x$ N(101 $\bar{A}$ ) surfaces. Applied Physics Letters, 2017, 110, .	3.3	5
41	Al $5+\hat{x}$ Si $5+\hat{x}$ N $12$ , a new Nitride compound. Scientific Reports, 2019, 9, 15907.	3.3	4
42	Theoretical modeling of growth processes, extended defects, and electronic properties of III $\hat{N}$ nitride semiconductor nanostructures. Physica Status Solidi (B): Basic Research, 2011, 248, 1837-1852.	1.5	3
43	Atomic scale morphology, growth behaviour and electronic properties of semipolar \$1\hat{x}\$Oar $\{1\}3\}$ \$ GaN surfaces. Journal of Physics Condensed Matter, 2013, 25, 045008.	1.8	3
44	Morphology and surface reconstructions of m-plane GaN. Materials Research Society Symposia Proceedings, 2002, 743, L4.1.1.	0.1	2
45	CHAPTER 9. Multi $\hat{s}$ cale Modelling of a Biological Material: The Arthropod Exoskeleton. RSC Smart Materials, 2013, , 197-218.	0.1	2
46	Quantum-Mechanical Study of Single-Crystalline and Polycrystalline Elastic Properties of Mg-Substituted Calcite Crystals. Key Engineering Materials, 0, 592-593, 335-341.	0.4	2
47	MEAM interatomic potentials of Ni, Re, and Ni $\hat{x}$ Re $\hat{x}$ Alloys for atomistic fracture simulations. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 015002.	2.0	2
48	Phase Transitions on Gan Surfaces. Materials Research Society Symposia Proceedings, 2002, 743, L3.9.1.	0.1	1
49	Strain-induced effects on the electronic structure and N K-edge ELNES of wurtzite AlN and Al $x$ Ga $1\hat{x}$ N. Journal of Physics: Conference Series, 2011, 326, 012016.	0.4	1
50	Phase diagram of grain boundary facet and line junctions in silicon. Physical Review Materials, 2020, 4, .	2.4	1
51	Efficient electronic passivation scheme for computing low-symmetry compound semiconductor surfaces in density-functional theory slab calculations. Physical Review Materials, 2021, 5, .	2.4	0
52	Scalable semipolar gallium nitride templates for high-speed LEDs. SPIE Newsroom, 0, , .	0.1	0