

Liverios Lymperakis

List of Publications by Year in descending order

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52
papers

1,873
citations

304743

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254184

43
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all docs

54
docs citations

54
times ranked

2706
citing authors

#	ARTICLE	IF	CITATIONS
1	MEAM interatomic potentials of Ni, Re, and Ni-Re Alloys for atomistic fracture simulations. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 015002.	2.0	2
2	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
3	Substitutional synthesis of sub-nanometer InGaN/GaN quantum wells with high indium content. Scientific Reports, 2021, 11, 20606.	3.3	9
4	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
5	Influence of strain on the indium incorporation in (0001) GaN. Physical Review Materials, 2020, 4, .	2.4	9
6	Phase diagram of grain boundary facet and line junctions in silicon. Physical Review Materials, 2020, 4, .	2.4	1
7	Role of hole confinement in the recombination properties of InGaN quantum structures. Scientific Reports, 2019, 9, 9047.	3.3	6
8	Al ₅ N ₂ Si ₅ , a new Nitride compound. Scientific Reports, 2019, 9, 15907.	3.3	4
9	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. Physical Review Letters, 2018, 121, 015702.	7.8	65
10	Ab-initio study of boron incorporation and compositional limits at GaN and AlN (0001) surfaces. AIP Advances, 2018, 8, .	1.3	10
11	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. Physical Review Materials, 2018, 2, .	2.4	36
12	Fermi-level pinning and intrinsic surface states of Al _{1-x} In _x N(101̂) surfaces. Applied Physics Letters, 2017, 110, .	3.3	5
13	Adsorption and desorption of hydrogen at nonpolar GaN surfaces: Kinetics and impact on surface vibrational and electronic properties. Physical Review B, 2017, 95, .	3.2	15
14	Selective-area growth of GaN nanowires on SiO ₂ -masked Si (111) substrates by molecular beam epitaxy. Journal of Applied Physics, 2016, 119, 224305.	2.5	29
15	Polarity in GaN and ZnO: Theory, measurement, growth, and devices. Applied Physics Reviews, 2016, 3, .	11.3	105
16	Development of semipolar (11-22) LEDs on GaN templates. Proceedings of SPIE, 2016, , .	0.8	8
17	Ab initio 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
18	Origin of the unusually strong luminescence of a-type screw dislocations in GaN. Physical Review B, 2014, 90, .	3.2	19

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19	Understanding and controlling indium incorporation and surface segregation on InGaN surfaces: An ab initio approach. Physical Review B, 2014, 89, .	3.2	47
20	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
21	Hidden surface states at non-polar GaN (101 $\bar{1}$) facets: Intrinsic pinning of nanowires. Applied Physics Letters, 2013, 103, .	3.3	45
22	Ab Initio Based conformational study of the crystalline β -chitin. Biopolymers, 2013, 99, 22-34.	2.4	27
23	Atomic scale morphology, growth behaviour and electronic properties of semipolar $\{10\bar{1}1\}$ GaN surfaces. Journal of Physics Condensed Matter, 2013, 25, 045008.	1.8	3
24	Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals. Journal of the Mechanical Behavior of Biomedical Materials, 2013, 20, 296-304.	3.1	32
25	CHAPTER 9. Multi-scale Modelling of a Biological Material: The Arthropod Exoskeleton. RSC Smart Materials, 2013, , 197-218.	0.1	2
26	Band offsets at zincblende-wurtzite GaAs nanowire sidewall surfaces. Applied Physics Letters, 2013, 103, .	3.3	28
27	Blocking Growth by an Electrically Active Subsurface Layer: The Effect of Si as an Antisurfactant in the Growth of GaN. Physical Review Letters, 2013, 110, 036103.	7.8	66
28	GaN(0001) surface states: Experimental and theoretical fingerprints to identify surface reconstructions. Physical Review B, 2013, 88, .	3.2	37
29	Reconstructions and electronic structure of (112 $\bar{2}$) and (112 $\bar{2}$) semipolar AlN surfaces. Journal of Applied Physics, 2012, 112, 033510.	2.5	7
30	Strain-induced effects on the electronic structure and N K-edge ELNES of wurtzite AlN and Al _x Ga _{1-x} N. Journal of Physics: Conference Series, 2011, 326, 012016.	0.4	1
31	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. European Physical Journal Plus, 2011, 126, 1.	2.6	22
32	Theoretical modeling of growth processes, extended defects, and electronic properties of III-nitride semiconductor nanostructures. Physica Status Solidi (B): Basic Research, 2011, 248, 1837-1852.	1.5	3
33	Hydrogen-enhanced local plasticity at dilute bulk H concentrations: The role of H-H interactions and the formation of local hydrides. Acta Materialia, 2011, 59, 2969-2980.	7.9	132
34	In situ scanning tunneling microscopy study of selective dissolution of Au ₃ Cu and Cu ₃ Au (001). Electrochimica Acta, 2011, 56, 1694-1700.	5.2	19
35	Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations. Journal of the Mechanical Behavior of Biomedical Materials, 2011, 4, 129-145.	3.1	91
36	Effect of edge threading dislocations on the electronic structure of InN. Applied Physics Letters, 2011, 98, .	3.3	23

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37	Electronic structure of $1/6\sqrt{3}$ partial dislocations in wurtzite GaN. <i>Journal of Applied Physics</i> , 2011, 109, .	2.5	16
38	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
39	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
40	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
41	Polar AlN/GaN interfaces: Structures and energetics. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2009, 206, 1892-1897.	1.8	20
42	Atomistic calculations on interfaces: Bridging the length and time scales. <i>European Physical Journal: Special Topics</i> , 2009, 177, 41-57.	2.6	9
43	Chemically ordered $\text{Al}_x\text{Ga}_{1-x}$ alloys: Spontaneous formation of natural quantum wells. <i>Physical Review B</i> , 2005, 71, .	3.2	53
44	Strain Induced Deep Electronic States around Threading Dislocations in GaN. <i>Physical Review Letters</i> , 2004, 93, 196401.	7.8	107
45	Gallium adsorption on (0001) GaN surfaces. <i>Physical Review B</i> , 2003, 67, .	3.2	131
46	A modified empirical potential for energetic calculations of planar defects in GaN. <i>Computational Materials Science</i> , 2003, 27, 43-49.	3.0	42
47	Morphology and surface reconstructions of GaN(11 $\bar{1}$,00) surfaces. <i>Applied Physics Letters</i> , 2003, 82, 1793-1795.	3.3	35
48	Phase Transitions on GaN Surfaces. <i>Materials Research Society Symposia Proceedings</i> , 2002, 743, L3.9.1.	0.1	1
49	Morphology and surface reconstructions of m-plane GaN. <i>Materials Research Society Symposia Proceedings</i> , 2002, 743, L4.1.1.	0.1	2
50	Atomic-scale models of interactions between inversion domain boundaries and intrinsic basal stacking faults in GaN. <i>Diamond and Related Materials</i> , 2002, 11, 905-909.	3.9	8
51	Quantum-Mechanical Study of Single-Crystalline and Polycrystalline Elastic Properties of Mg-Substituted Calcite Crystals. <i>Key Engineering Materials</i> , 0, 592-593, 335-341.	0.4	2
52	Scalable semipolar gallium nitride templates for high-speed LEDs. <i>SPIE Newsroom</i> , 0, , .	0.1	0