PaweÅ, Kempisty

List of Publications by Year
in descending order

61	895	394421	552781
papers	citations	19	26
		h-index	g-index

64	64	64	680
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electrostatic condition for the termination of the opposite face of the slab in density functional theory simulations of semiconductor surfaces. Journal of Applied Physics, 2009, 105, .	2.5	46
2	Ab initio studies of electronic properties of bare GaN(0001) surface. Journal of Applied Physics, 2009, 106, .	2.5	43
3	Ab initio determination of atomic structure and energy of surface states of bare and hydrogen covered GaN (0001) surface â€" Existence of the Surface States Stark Effect (SSSE). Surface Science, 2011, 605, 695-713.	1.9	36
4	Fermi level influence on the adsorption at semiconductor surfacesâ€"ab initio simulations. Journal of Applied Physics, 2013, 114, .	2.5	35
5	Principal physical properties of GaN/AlN multiquantum well systems determined by density functional theory calculations. Journal of Applied Physics, 2013, 113, .	2.5	32
6	Foundations of ab initio simulations of electric charges and fields at semiconductor surfaces within slab models. Journal of Applied Physics, 2013, 114, .	2.5	32
7	On the nature of Surface States Stark Effect at clean GaN(0001) surface. Journal of Applied Physics, 2012, 112, .	2.5	31
8	Homoepitaxial growth of HVPE-GaN doped with Si. Journal of Crystal Growth, 2016, 456, 91-96.	1.5	29
9	Evolution of the free energy of the GaN(0001) surface based on first-principles phonon calculations. Physical Review B, 2019, 100, .	3.2	29
10	Contactless electroreflectance studies of the Fermi level position at the air/GaN interface: Bistable nature of the Ga-polar surface. Applied Surface Science, 2017, 396, 1657-1666.	6.1	27
11	Thermodynamic analysis of (0001) and $(000ar{1})$ GaN metalorganic vapor phase epitaxy. Japanese Journal of Applied Physics, 2017, 56, 070304.	1.5	27
12	Influence of hydrogen and TMIn on indium incorporation in MOVPE growth of InGaN layers. Journal of Crystal Growth, 2014, 402, 330-336.	1.5	26
13	Density Functional Theory (DFT) Simulations and Polarization Analysis of the Electric Field in InN/GaN Multiple Quantum Wells (MQWs). Journal of Physical Chemistry C, 2010, 114, 14410-14416.	3.1	24
14	CFD and reaction computational analysis of the growth of GaN by HVPE method. Journal of Crystal Growth, 2006, 296, 31-42.	1.5	23
15	Adsorption of ammonia at GaN(0001) surface in the mixed ammonia/hydrogen ambient - a summary of ab initio data. AIP Advances, 2014, 4, .	1.3	23
16	Ab initio and experimental studies of polarization and polarization related fields in nitrides and nitride structures. AIP Advances, 2017, 7, .	1.3	23
17	High pressureâ€"high temperature seeded growth of GaN on 1 in sapphire/GaN templates: Analysis of convective transport. Journal of Crystal Growth, 2007, 307, 259-267.	1.5	21
18	Fermi level pinning and the charge transfer contribution to the energy of adsorption at semiconducting surfaces. Journal of Applied Physics, 2014, 115, 043529.	2.5	21

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19	Ab initio investigation of adsorption of atomic and molecular hydrogen at GaN(0001) surface. Journal of Crystal Growth, 2012, 358, 64-74.	1.5	19
20	Ab initio determination of electron affinity of polar nitride surfaces, clean and under Cs coverage. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	2.1	19
21	DFT modeling of carbon incorporation in GaN(0001) and GaN(0001Â¯) metalorganic vapor phase epitaxy. Applied Physics Letters, 2017, 111, .	3.3	19
22	Thermodynamic and kinetic approach in density functional theory studies of microscopic structure of GaN(0001) surface in ammonia-rich conditions. Journal of Chemical Physics, 2008, 129, 234705.	3.0	18
23	Structural and electronic properties of AlN(0001) surface under partial N coverage as determined by ab initio approach. Journal of Applied Physics, 2015, 118, .	2.5	16
24	Review: GaN growth by ammonia based methods â€“ density functional theory study. Crystal Research and Technology, 2009, 44, 1038-1046.	1.3	15
25	Thermodynamic foundations of applications of ab initio methods for determination of the adsorbate equilibria: hydrogen at the GaN(0001) surface. Physical Chemistry Chemical Physics, 2017, 19, 29676-29684.	2.8	14
26	Modelling the growth of nitrides in ammoniaâ€rich environment. Crystal Research and Technology, 2007, 42, 1281-1290.	1.3	12
27	Crystal growth of GaN on (0001) face by HVPE-atomistic scale simulation. Journal of Crystal Growth, 2007, 303, 37-43.	1.5	12
28	Density Functional Theory Determination of Structural and Electronic Properties of Struvite. Journal of Physical Chemistry A, 2010, 114, 7800-7808.	2.5	12
29	Advances in modeling semiconductor epitaxy: Contributions of growth orientation and surface reconstruction to InN metalorganic vapor phase epitaxy. Applied Physics Express, 2016, 9, 125601.	2.4	12
30	Thermodynamics of GaN(s)-NH 3 (v)+N 2 (v)+H 2 (v) system â€“ Electronic aspects of the processes at GaN(0001) surface. Surface Science, 2017, 662, 12-33.	1.9	12
31	DFT study on point defects migration through the pseudomorphic and lattice-matched InN/GaN interfaces. Computational Materials Science, 2021, 186, 110039.	3.0	12
32	Crystal growth of GaN on (0001) face by HVPE: Ab initio simulations. Journal of Crystal Growth, 2008, 310, 900-905.	1.5	11
33	General aspects of the vapor growth of semiconductor crystals â€“ A study based on DFT simulations of the NH3/NH2 covered GaN(0001) surface in hydrogen ambient. Journal of Crystal Growth, 2014, 390, 71-79.	1.5	11
34	CH4 Adsorption Probability on GaN(0001) and (000â¯1) during Metalorganic Vapor Phase Epitaxy and Its Relationship to Carbon Contamination in the Films. Materials, 2019, 12, 972.	2.9	10
35	Ab initio study of the properties of GaN(0001) surface at MOVPE and HVPE growth conditions. Physica Status Solidi C: Current Topics in Solid State Physics, 2012, 9, 826-829.	0.8	9
36	Adsorption of N2 and H2 at AlN(0001) Surface: Ab Initio Assessment of the Initial Stage of Ammonia Catalytic Synthesis. Journal of Physical Chemistry C, 2018, 122, 20301-20311.	3.1	9

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37	Progress in Modeling Compound Semiconductor Epitaxy: Unintentional Doping in GaN MOVPE. Crystal Growth and Design, 2021, 21, 1878-1890.	3.0	9
38	Chemical inactivity of GaN(0001) surface â€“ The role of oxygen adsorption â€“ Ab initio picture. Materials Science in Semiconductor Processing, 2019, 91, 252-259.	4.0	8
39	Effects of Mg dopant in Al-composition-graded Al_xGa_{1â^'x}N (0.45Ââ‰Âx) on vertical electrical conductivity of ultrawide bandgap AlGaN pâ€“n junction. Applied Physics Express, 2021, 14, 096503.	2.4	8
40	Adsorption of ammonia on hydrogen covered GaN(0001) surface â€“ Density Functional Theory study. Journal of Crystal Growth, 2014, 401, 514-517.	1.5	7
41	Role of chlorine in the dynamics of GaN(0001) surface during HVPE GaN growthâ€”Ab initio study. Journal of Crystal Growth, 2008, 310, 1391-1397.	1.5	6
42	DFT study of ammonia desorption from the GaN(0001) surface covered with a NH3/NH2 mixture. Journal of Crystal Growth, 2014, 403, 105-109.	1.5	6
43	Critical Evaluation of Various Spontaneous Polarization Models and Induced Electric Fields in III-Nitride Multi-Quantum Wells. Materials, 2021, 14, 4935.	2.9	6
44	Modeling of the Point Defect Migration across the AlN/GaN Interfacesâ€”Ab Initio Study. Materials, 2022, 15, 478.	2.9	6
45	Ab initiostudy of Ga-GaN system: Transition from adsorbed metal atoms to a metalâ€“semiconductor junction. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, 061101.	2.1	5
46	Adsorption of gallium on GaN(0001) surface in ammonia-rich conditions: A new effect associated with the Fermi level position. Journal of Crystal Growth, 2014, 401, 78-81.	1.5	4
47	Dissipation of the excess energy of the adsorbate-thermalization via electron transfer. Physical Chemistry Chemical Physics, 2017, 19, 9149-9155.	2.8	4
48	Catalytic Synthesis of Nitric Monoxide at the AlN(0001) Surface: Ab Initio Analysis. Journal of Physical Chemistry C, 2019, 123, 10893-10906.	3.1	4
49	Ab initio and thermodynamic picture of Al adsorption of AlN(0001) surface â€“ Role of bond creation and electron transition contributions. Applied Surface Science, 2020, 532, 147419.	6.1	4
50	Electronic and structural properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>:</mml:mo><mml:mi>Cu</mml:mi></mml:mrow></m	2.4	4
51	On the composite discontinuous Galerkin method for simulations of electric properties of semiconductor devices. Electronic Transactions on Numerical Analysis, 0, 51, 75-98.	0.0	4
52	Suppressing the lateral growth during HVPE-GaN crystallization in the c-direction. Journal of Crystal Growth, 2021, 556, 125986.	1.5	3
53	Investigation of beryllium diffusion in HVPE-GaN grown in [11â€“20] and [10-10] crystallographic directions. Materials Science in Semiconductor Processing, 2022, 139, 106332.	4.0	3
54	Mass flow and reaction analysis of the growth of GaN by HVPE. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 131-134.	1.8	2

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55	DFT modeling of AlN/GaN multi-quantum wells. Physica Status Solidi C: Current Topics in Solid State Physics, 2013, 10, 323-326.	0.8	2
56	Doping effects in InN/GaN short-period quantum well structuresâ€"Theoretical studies based on density functional methods. Journal of Crystal Growth, 2014, 401, 652-656.	1.5	2
57	Liquid phase epitaxy of GaN on MOCVD GaN/sapphire and HVPE freeâ€standing substrates under high nitrogen pressure. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 1539-1542.	0.8	1
58	Discretization of the Drift-Diffusion Equations with the Composite Discontinuous Galerkin Method. Lecture Notes in Computer Science, 2016, , 391-400.	1.3	1
59	Facet stability of GaN during tri-halide vapor phase epitaxy: an ab initio-based approach. CrystEngComm, 2021, 23, 1423-1428.	2.6	0
60	Al coverage of AlN(0001) surface and Al vapor pressure â€“ Thermodynamic assessment based on ab initio calculations. Computational Materials Science, 2022, 203, 111159.	3.0	0
61	DFT modeling of unintentional oxygen incorporation enhanced by magnesium in GaN(0001) and AlN(0001) growth surfaces during metalorganic vapor phase epitaxy. Physica Status Solidi (B): Basic Research, 0, , .	1.5	0