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	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
2	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
3	Modeling of the Point Defect Migration across the AlN/GaN Interfacesâ€”Ab Initio Study. Materials, 2022, 15, 478.	2.9	6
4	DFT study on point defects migration through the pseudomorphic and lattice-matched InN/GaN interfaces. Computational Materials Science, 2021, 186, 110039.	3.0	12
5	Facet stability of GaN during tri-halide vapor phase epitaxy: an ab initio-based approach. CrystEngComm, 2021, 23, 1423-1428.	2.6	0
6	Progress in Modeling Compound Semiconductor Epitaxy: Unintentional Doping in GaN MOVPE. Crystal Growth and Design, 2021, 21, 1878-1890.	3.0	9
7	Suppressing the lateral growth during HVPE-GaN crystallization in the c-direction. Journal of Crystal Growth, 2021, 556, 125986.	1.5	3
8	Critical Evaluation of Various Spontaneous Polarization Models and Induced Electric Fields in III-Nitride Multi-Quantum Wells. Materials, 2021, 14, 4935.	2.9	6
9	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
10	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
11	Evolution of the free energy of the GaN(0001) surface based on first-principles phonon calculations. Physical Review B, 2019, 100, .	3.2	29
12	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
13	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
14	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
15	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
16	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></	2.4	4
17	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
18	Ab initio and experimental studies of polarization and polarization related fields in nitrides and nitride structures. AIP Advances, 2017, 7, .	1.3	23

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19	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
20	Dissipation of the excess energy of the adsorbate-thermalization via electron transfer. Physical Chemistry Chemical Physics, 2017, 19, 9149-9155.	2.8	4
21	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
22	DFT modeling of carbon incorporation in GaN(0001) and GaN(0001Â¯) metalorganic vapor phase epitaxy. Applied Physics Letters, 2017, 111, .	3.3	19
23	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
24	Thermodynamic analysis of (0001) and $(000ar{1})$ GaN metalorganic vapor phase epitaxy. Japanese Journal of Applied Physics, 2017, 56, 070304.	1.5	27
25	Discretization of the Drift-Diffusion Equations with the Composite Discontinuous Galerkin Method. Lecture Notes in Computer Science, 2016, , 391-400.	1.3	1
26	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
27	Homoepitaxial growth of HVPE-GaN doped with Si. Journal of Crystal Growth, 2016, 456, 91-96.	1.5	29
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	Fermi level influence on the adsorption at semiconductor surfacesâ€"ab initio simulations. Journal of Applied Physics, 2013, 114, .	2.5	35
39	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
40	Principal physical properties of GaN/AlN multiquantum well systems determined by density functional theory calculations. Journal of Applied Physics, 2013, 113, .	2.5	32
41	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
42	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
43	On the nature of Surface States Stark Effect at clean GaN(0001) surface. Journal of Applied Physics, 2012, 112, .	2.5	31
44	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
45	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
46	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
47	Density Functional Theory Determination of Structural and Electronic Properties of Struvite. Journal of Physical Chemistry A, 2010, 114, 7800-7808.	2.5	12
48	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
49	Review: GaN growth by ammonia based methods â€“ density functional theory study. Crystal Research and Technology, 2009, 44, 1038-1046.	1.3	15
50	Ab initio studies of electronic properties of bare GaN(0001) surface. Journal of Applied Physics, 2009, 106, .	2.5	43
51	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
52	Crystal growth of GaN on (0001) face by HVPE: Ab initio simulations. Journal of Crystal Growth, 2008, 310, 900-905.	1.5	11
53	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
54	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

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55	Modelling the growth of nitrides in ammoniaâ€rich environment. Crystal Research and Technology, 2007, 42, 1281-1290.	1.3	12
56	Crystal growth of GaN on (0001) face by HVPE-atomistic scale simulation. Journal of Crystal Growth, 2007, 303, 37-43.	1.5	12
57	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
58	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
59	CFD and reaction computational analysis of the growth of GaN by HVPE method. Journal of Crystal Growth, 2006, 296, 31-42.	1.5	23
60	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
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