List of Publications by Year in descending order

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DANNEL KEMDISTY

#	Article	IF	CITATIONS
1	Investigation of beryllium diffusion in HVPE-GaN grown in [11–20] and [10-10] crystallographic directions. Materials Science in Semiconductor Processing, 2022, 139, 106332.	1.9	3
2	Al coverage of AlN(0001) surface and Al vapor pressure – Thermodynamic assessment based on ab initio calculations. Computational Materials Science, 2022, 203, 111159.	1.4	0
3	Modeling of the Point Defect Migration across the AlN/GaN Interfaces—Ab Initio Study. Materials, 2022, 15, 478.	1.3	6
4	DFT study on point defects migration through the pseudomorphic and lattice-matched InN/GaN interfaces. Computational Materials Science, 2021, 186, 110039.	1.4	12
5	Facet stability of GaN during tri-halide vapor phase epitaxy: an ab initio-based approach. CrystEngComm, 2021, 23, 1423-1428.	1.3	Ο
6	Progress in Modeling Compound Semiconductor Epitaxy: Unintentional Doping in GaN MOVPE. Crystal Growth and Design, 2021, 21, 1878-1890.	1.4	9
7	Suppressing the lateral growth during HVPE-GaN crystallization in the c-direction. Journal of Crystal Growth, 2021, 556, 125986.	0.7	3
8	Critical Evaluation of Various Spontaneous Polarization Models and Induced Electric Fields in III-Nitride Multi-Quantum Wells. Materials, 2021, 14, 4935.	1.3	6
9	Effects of Mg dopant in Al-composition-graded Al <sub> x </sub> Ga <sub>1â~'x </sub> N (0.45Â≤̂x) on vertical electrical conductivity of ultrawide bandgap AlGaN p–n junction. Applied Physics Express, 2021, 14, 096503.	1.1	8
10	Ab initio and thermodynamic picture of Al adsorption of AlN(0001) surface – Role of bond creation and electron transition contributions. Applied Surface Science, 2020, 532, 147419.	3.1	4
11	Evolution of the free energy of the GaN(0001) surface based on first-principles phonon calculations. Physical Review B, 2019, 100, .	1.1	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.	1.3	10
13	Catalytic Synthesis of Nitric Monoxide at the AlN(0001) Surface: Ab Initio Analysis. Journal of Physical Chemistry C, 2019, 123, 10893-10906.	1.5	4
14	Chemical inactivity of GaN(0001) surface – The role of oxygen adsorption – Ab initio picture. Materials Science in Semiconductor Processing, 2019, 91, 252-259.	1.9	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. Electronic and structural properties of complements	1.5	9
16	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	0.9	4
17	mathvariant="normal">e <mml:mn>3</mml:mn> <mml:mo>:</mml:mo> : <mml:mi>Cu<i>Ab initio</i> 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, .</mml:mi>	nml:mi> <br 0.9	mml:mrow><  19
18	<i>Ab initio</i> and experimental studies of polarization and polarization related fields in nitrides and nitride structures. AIP Advances, 2017, 7, .	0.6	23

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19	Thermodynamics of GaN(s)-NH 3 (v)+N 2 (v)+H 2 (v) system – Electronic aspects of the processes at GaN(0001) surface. Surface Science, 2017, 662, 12-33.	0.8	12
20	Dissipation of the excess energy of the adsorbate-thermalization via electron transfer. Physical Chemistry Chemical Physics, 2017, 19, 9149-9155.	1.3	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.	3.1	27
22	DFT modeling of carbon incorporation in GaN(0001) and GaN(0001Â⁻) metalorganic vapor phase epitaxy. Applied Physics Letters, 2017, 111, .	1.5	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.	1.3	14
24	Thermodynamic analysis of (0001) and \$(000ar{1})\$ GaN metalorganic vapor phase epitaxy. Japanese Journal of Applied Physics, 2017, 56, 070304.	0.8	27
25	Discretization of the Drift-Diffusion Equations with the Composite Discontinuous Galerkin Method. Lecture Notes in Computer Science, 2016, , 391-400.	1.0	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.	1.1	12
27	Homoepitaxial growth of HVPE-GaN doped with Si. Journal of Crystal Growth, 2016, 456, 91-96.	0.7	29
28	Ab initiostudy of Ga-GaN system: Transition from adsorbed metal atoms to a metal–semiconductor junction. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, 061101.	0.9	5
29	Structural and electronic properties of AlN(0001) surface under partial N coverage as determined by <i>ab initio</i> approach. Journal of Applied Physics, 2015, 118, .	1.1	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, .	0.6	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.	1.1	21
32	Doping effects in InN/GaN short-period quantum well structures—Theoretical studies based on density functional methods. Journal of Crystal Growth, 2014, 401, 652-656.	0.7	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.	0.7	4
34	General aspects of the vapor growth of semiconductor crystals – 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.	0.7	11
35	Influence of hydrogen and TMIn on indium incorporation in MOVPE growth of InGaN layers. Journal of Crystal Growth, 2014, 402, 330-336.	0.7	26
36	Adsorption of ammonia on hydrogen covered GaN(0001) surface – Density Functional Theory study. Journal of Crystal Growth, 2014, 401, 514-517.	0.7	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.	0.7	6
38	Fermi level influence on the adsorption at semiconductor surfaces— <i>ab initio</i> simulations. Journal of Applied Physics, 2013, 114, .	1.1	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, .	1.1	32
41	Foundations of <i>ab initio</i> simulations of electric charges and fields at semiconductor surfaces within slab models. Journal of Applied Physics, 2013, 114, .	1.1	32
42	Ab initio investigation of adsorption of atomic and molecular hydrogen at GaN(0001) surface. Journal of Crystal Growth, 2012, 358, 64-74.	0.7	19
43	On the nature of Surface States Stark Effect at clean GaN(0001) surface. Journal of Applied Physics, 2012, 112, .	1.1	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 — Existence of the Surface States Stark Effect (SSSE). Surface Science, 2011, 605, 695-713.	0.8	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.	1.5	24
47	Density Functional Theory Determination of Structural and Electronic Properties of Struvite. Journal of Physical Chemistry A, 2010, 114, 7800-7808.	1.1	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, .	1.1	46
49	Review: GaN growth by ammonia based methods – density functional theory study. Crystal Research and Technology, 2009, 44, 1038-1046.	0.6	15
50	<i>Ab initio</i> studies of electronic properties of bare GaN(0001) surface. Journal of Applied Physics, 2009, 106, .	1.1	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.	0.7	11
53	Role of chlorine in the dynamics of GaN(0001) surface during HVPE GaN growth—Ab initio study. Journal of Crystal Growth, 2008, 310, 1391-1397.	0.7	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	1.2	18

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55	Modelling the growth of nitrides in ammoniaâ€rich environment. Crystal Research and Technology, 2007, 42, 1281-1290.	0.6	12
56	Crystal growth of GaN on (0001) face by HVPE-atomistic scale simulation. Journal of Crystal Growth, 2007, 303, 37-43.	0.7	12
57	High pressure–high temperature seeded growth of GaN on 1 in sapphire/GaN templates: Analysis of convective transport. Journal of Crystal Growth, 2007, 307, 259-267.	0.7	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.	0.8	2
59	CFD and reaction computational analysis of the growth of GaN by HVPE method. Journal of Crystal Growth, 2006, 296, 31-42.	0.7	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, , .	0.7	0