JÃ¼rgen FurthmÃ¼ller

List of Publications by Year
in descending order

76 papers	59,448 citations	117625 34 h-index	71685 76 g-index
78 all docs	78 docs citations	78 times ranked	45563 citing authors

#	Article	IF	Citations
1	Efficient strain-induced light emission in lonsdaleite germanium. Physical Review Materials, 2021, 5, .	2.4	16
2	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. Physical Review Materials, 2021, 5, .	2.4	7
3	Influence of Polymorphism on the Electronic Structure of Ga₂O₃. Chemistry of Materials, 2020, 32, 8460-8470.	6.7	35
4	Electronic and Optical Properties of Small Metal Fluoride Clusters. ACS Omega, 2020, 5, 13268-13277.	3.5	8
5	Direct-bandgap emission from hexagonal Ge and SiGe alloys. Nature, 2020, 580, 205-209.	27.8	231
6	Towards a photonic band edge laser using hexagonal-SiGe nanowire arrays (Conference Presentation). , 2020, , .		1
7	Influence of screening dynamics on excitons in Ga2O3 polymorphs. Applied Physics Letters, 2019, 114, .	3.3	20
8	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. Physical Review B, 2019, 100, .	3.2	25
9	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. Physical Review Materials, 2019, 3, .	2.4	41
10	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. Physical Review B, 2016, 94, .	3.2	24
11	Dielectric tensor of monoclinic Ga₂O₃ single crystals in the spectral range 0.5â€“8.5 eV. APL Materials, 2015, 3, 106106.	5.1	81
12	One- and two-particle effects in the electronic and optical spectra of barium fluoride. Journal of Physics Condensed Matter, 2014, 26, 125501.	1.8	6
13	Structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-tin nanocrystals from first principles. Physical Review B, 2013, 87, .	3.2	29
14	Electronic and optical properties of cadmium fluoride: The role of many-body effects. Physical Review B, 2013, 87, .	3.2	20
15	Ab initiocalculation of optical properties with excitonic effects in wurtzite InxGa1âˆ’xN and InxAl1âˆ’xN alloys. Physical Review B, 2013, 87, .	3.2	14
16	Optical absorption and emission of Î±-Sn nanocrystals from first principles. Nanotechnology, 2013, 24, 405702.	2.6	13
17	In4d and Ga3d levels in In_xX_{1âˆ’}_xN (Xâ€‰=â€‰Ga, Al) alloys. Applied Physics Letters, 2013, 102, 172105.	3.3	2
18	Electronic bands of III-V semiconductor polytypes and their alignment. Physical Review B, 2012, 86, .	3.2	134

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19	Substitution of cations in wurtzitic In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N and In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N alloys. Physical Review B, 2009, 80, .	3.2	22
20	GaMnAs: Position of Mn-d levels and majority spin band gap predicted from GGA-1/2 calculations. Applied Physics Letters, 2012, 100, .	3.3	26
21	Electronic and optical properties of Mg_xZn_{1â^’x}O and Cd_xZn_{1â^’x}O fromab initiocalculations. New Journal of Physics, 2011, 13, 085012.	2.9	60
22	Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach. Applied Physics Letters, 2011, 98, .	3.3	141
23	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. Physical Review B, 2011, 84, .	3.2	5
24	Spin-orbit effects in structural and electronic properties for the solid state of the group-14 elements from carbon to superheavy element 114. Physical Review B, 2010, 82, .	3.2	61
25	Bandâ€structure and opticalâ€transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 2150-2153.	1.5	68
26	Structural features and electronic properties of group-III-, group-IV-, and group-V-doped Si nanocrystallites. Journal of Physics Condensed Matter, 2007, 19, 466211.	1.8	37
27	Strain influence on valence-band ordering and excitons in ZnO: Anab initiostudy. Applied Physics Letters, 2007, 91, 241915.	3.3	55
28	Nonparabolicity and excitons in optical absorption of InN. Journal of Crystal Growth, 2006, 288, 294-297.	1.5	5
29	INFLUENCE OF STRUCTURAL RELAXATION ON THE OPTICAL AND ELECTRONIC PROPERTIES OF Ge and Si NANOCRYSTALS. , 2005, , .		0
30	Band structure and electron gas of In chains on Si(111). Surface Science, 2005, 589, 77-90.	1.9	12
31	Quasiparticle and excitonic effects in the optical spectra of diamond, SiC, Si, GaP, GaAs, InP, and AlN. Physica Status Solidi (B): Basic Research, 2005, 242, 2720-2728.	1.5	22
32	Optical properties of Si and Ge nanocrystals: Parameter-free calculations. Physica Status Solidi (B): Basic Research, 2005, 242, 3053-3063.	1.5	35
33	Classical versus ab initio structural relaxation: electronic excitations and optical properties of Ge nanocrystals embedded in an SiC matrix. Journal of Physics Condensed Matter, 2005, 17, 643-651.	1.8	1
34	Influence of oxygen on optical properties of Si nanocrystallites. Applied Physics Letters, 2005, 87, 143113.	3.3	25
35	Magnetic properties of MnN: Influence of strain and crystal structure. Applied Physics Letters, 2005, 86, 164105.	3.3	28
36	Electron correlation effects on SiC(111) and SiC(0001) surfaces. Journal of Physics Condensed Matter, 2004, 16, S1721-S1732.	1.8	28

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37	Energy gap and optical properties of InxGa1xN. Physica Status Solidi A, 2003, 195, 628-633.	1.7	92
38	Lattice parameter and energy band gap of cubic AlxGayIn1â^'xâ^'yN quaternary alloys. Applied Physics Letters, 2003, 83, 890-892.	3.3	69
39	Gap bowing and Stokes shift in InxGa1â^'xN alloys: First-principles studies. Applied Physics Letters, 2002, 80, 1394-1396.	3.3	45
40	Spinodal decomposition in BxGa1â^'xN and BxAl1â^'xN alloys. Applied Physics Letters, 2002, 80, 1177-1179.	3.3	41
41	Phase diagram, chemical bonds, and gap bowing of cubic InxAl1â^'xN alloys:Abâ€‰initiocalculations. Journal of Applied Physics, 2002, 92, 7109-7113.	2.5	32
42	Phase Separation, Gap Bowing, and Structural Properties of Cubic InxAl1â€"xN. Physica Status Solidi (B): Basic Research, 2002, 234, 956-960.	1.5	12
43	Do we know the fundamental energy gap of InN?. Journal of Crystal Growth, 2002, 246, 315-319.	1.5	117
44	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. Applied Physics Letters, 2002, 80, 769-771.	3.3	102
45	On the nature of the D1-defect center in SiC: A photoluminescence study of layers grown by solid-source molecular-beam epitaxy. Applied Physics Letters, 2001, 78, 2512-2514.	3.3	39
46	Native defects and complexes in SiC. Journal of Physics Condensed Matter, 2001, 13, 9027-9037.	1.8	18
47	Dielectric and lattice-dynamical properties of III-nitrides. Journal of Electronic Materials, 2000, 29, 281-284.	2.2	4
48	First-principles calculations of the thermodynamic and structural properties of strainedInxGa1â^'xNandAlxGa1â^'xNalloys. Physical Review B, 2000, 62, 2475-2485.	3.2	187
49	Intravacancy transition energies in3Câ^'and4Hâ^'SiC. Physical Review B, 2000, 61, 13655-13658.	3.2	15
50	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. Physical Review B, 2000, 62, 6854-6857.	3.2	63
51	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row andd-electron elements. Physical Review B, 2000, 61, 4576-4587.	3.2	102
52	Dynamics and polarization of group-III nitride lattices:â€‚A first-principles study. Physical Review B, 2000, 62, 8003-8011.	3.2	108
53	Initial stages of III-nitride growth. Applied Physics Letters, 1999, 74, 3851-3853.	3.3	21
54	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. Physical Review B, 1999, 59, 15166-15180.	3.2	225

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55	Surface Energies and Surface Dipoles at III-Nitride(111) Surfaces in Dependence on Stoichiometry. Physica Status Solidi (B): Basic Research, 1999, 216, 675-678.	1.5	11
56	Polytypic transformations in SiC: Anab initiostudy. Physical Review B, 1999, 60, 13261-13264.	3.2	23
57	High-precision determination of atomic positions in crystals: The case of6H- and4H-SiC. Physical Review B, 1998, 57, 2647-2650.	3.2	110
58	Theoretical investigation of edge dislocations in AlN. Applied Physics Letters, 1998, 72, 3467-3469.	3.3	42
59	Si-richSiC(111)/(0001)3Ã—3and3Ã—3surfaces: A Mott-Hubbard picture. Physical Review B, 1998, 58, 13712-13716.	3.2	73
60	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. Physical Review B, 1998, 58, R1722-R1725.	3.2	67
61	Stacking faults in group-IV crystals: Anab initiostudy. Physical Review B, 1998, 58, 1326-1330.	3.2	85
62	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination ofSiC(111)-(3Ã—3). Physical Review Letters, 1998, 80, 758-761.	7.8	170
63	Carbon vacancy in SiC: A negative- U system. Europhysics Letters, 1998, 44, 309-314.	2.0	17
64	Polytypism and surface structure of SiC. Diamond and Related Materials, 1997, 6, 1346-1348.	3.9	16
65	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. Physical Review B, 1997, 56, 15629-15646.	3.2	324
66	Structural and electronic properties of rhodium surfaces: an ab initio approach. Surface Science, 1996, 346, 300-321.	1.9	118
67	Stoichiometry and surface reconstructions of (001) surfaces of silicon carbide. Surface Science, 1996, 352-354, 55-59.	1.9	12
68	Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Computational Materials Science, 1996, 6, 15-50.	3.0	54,900
69	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. Europhysics Letters, 1995, 32, 729-734.	2.0	663
70	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. Europhysics Letters, 1994, 28, 659-664.	2.0	62
71	Are amorphous ferromagnets with Î»S=0 magnetostrictive on a local scale?. Applied Physics Letters, 1991, 59, 2049-2051.	3.3	9
72	Local magnetic anisotropy and magnetostriction of amorphous ferromagnets. Physica B: Condensed Matter, 1990, 161, 225-231.	2.7	13

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73	Theory of atomic level magnetostrictive deformations and stresses in amorphous ferromagnets. Journal of Magnetism and Magnetic Materials, 1988, 75, 225-232.	2.3	14
74	Various contributions to magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1988, 72, 6-12.	2.3	11
75	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1987, 69, 79-88.	2.3	44
76	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1987, 69, 89-98.	2.3	26