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	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
2	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. Europhysics Letters, 1995, 32, 729-734.	2.0	663
3	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. Physical Review B, 1997, 56, 15629-15646.	3.2	324
4	Direct-bandgap emission from hexagonal Ge and SiGe alloys. Nature, 2020, 580, 205-209.	27.8	231
5	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. Physical Review B, 1999, 59, 15166-15180.	3.2	225
6	First-principles calculations of the thermodynamic and structural properties of strainedInxGa1â^'xNandAlxGa1â^'xNalloys. Physical Review B, 2000, 62, 2475-2485.	3.2	187
7	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
8	Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach. Applied Physics Letters, 2011, 98, .	3.3	141
9	Electronic bands of III-V semiconductor polytypes and their alignment. Physical Review B, 2012, 86, .	3.2	134
10	Structural and electronic properties of rhodium surfaces: an ab initio approach. Surface Science, 1996, 346, 300-321.	1.9	118
11	Do we know the fundamental energy gap of InN?. Journal of Crystal Growth, 2002, 246, 315-319.	1.5	117
12	High-precision determination of atomic positions in crystals: The case of6H- and4H-SiC. Physical Review B, 1998, 57, 2647-2650.	3.2	110
13	Dynamics and polarization of group-III nitride lattices:â€‚A first-principles study. Physical Review B, 2000, 62, 8003-8011.	3.2	108
14	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
15	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. Applied Physics Letters, 2002, 80, 769-771.	3.3	102
16	Energy gap and optical properties of InxGa1xN. Physica Status Solidi A, 2003, 195, 628-633.	1.7	92
17	Stacking faults in group-IV crystals: Anab initiostudy. Physical Review B, 1998, 58, 1326-1330.	3.2	85
18	Dielectric tensor of monoclinic Ga₂O₃ single crystals in the spectral range 0.5â€“8.5 eV. APL Materials, 2015, 3, 106106.	5.1	81

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19	Si-richSiC(111)/(0001)3Ã—3and3Ã—3surfaces: A Mott-Hubbard picture. Physical Review B, 1998, 58, 13712-13716.	3.2	73
20	Lattice parameter and energy band gap of cubic AlxGayIn1â^'xâ^'yN quaternary alloys. Applied Physics Letters, 2003, 83, 890-892.	3.3	69
21	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
22	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. Physical Review B, 1998, 58, R1722-R1725.	3.2	67
23	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. Physical Review B, 2000, 62, 6854-6857.	3.2	63
24	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. Europhysics Letters, 1994, 28, 659-664.	2.0	62
25	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
26	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
27	Strain influence on valence-band ordering and excitons in ZnO: Anab initiostudy. Applied Physics Letters, 2007, 91, 241915.	3.3	55
28	Gap bowing and Stokes shift in InxGa1â^'xN alloys: First-principles studies. Applied Physics Letters, 2002, 80, 1394-1396.	3.3	45
29	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1987, 69, 79-88.	2.3	44
30	Theoretical investigation of edge dislocations in AlN. Applied Physics Letters, 1998, 72, 3467-3469.	3.3	42
31	Spinodal decomposition in BxGa1â^'xN and BxAl1â^'xN alloys. Applied Physics Letters, 2002, 80, 1177-1179.	3.3	41
32	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. Physical Review Materials, 2019, 3, .	2.4	41
33	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
34	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
35	Optical properties of Si and Ge nanocrystals: Parameter-free calculations. Physica Status Solidi (B): Basic Research, 2005, 242, 3053-3063.	1.5	35
36	Influence of Polymorphism on the Electronic Structure of Ga₂O₃. Chemistry of Materials, 2020, 32, 8460-8470.	6.7	35

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37	Phase diagram, chemical bonds, and gap bowing of cubic InxAl1âˆ’xN alloys:Abâ€‰initiocalculations. Journal of Applied Physics, 2002, 92, 7109-7113.	2.5	32
38	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
39	Electron correlation effects on SiC(111) and SiC(0001) surfaces. Journal of Physics Condensed Matter, 2004, 16, S1721-S1732.	1.8	28
40	Magnetic properties of MnN: Influence of strain and crystal structure. Applied Physics Letters, 2005, 86, 164105.	3.3	28
41	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1987, 69, 89-98.	2.3	26
42	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
43	Influence of oxygen on optical properties of Si nanocrystallites. Applied Physics Letters, 2005, 87, 143113.	3.3	25
44	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. Physical Review B, 2019, 100, .	3.2	25
45	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. Physical Review B, 2016, 94, .	3.2	24
46	Polytypic transformations in SiC: Anab initiostudy. Physical Review B, 1999, 60, 13261-13264.	3.2	23
47	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
48	Distribution 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>âˆ’</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:mat. Physical Revie	3.2	22
49	Initial stages of III-nitride growth. Applied Physics Letters, 1999, 74, 3851-3853.	3.3	21
50	Electronic and optical properties of cadmium fluoride: The role of many-body effects. Physical Review B, 2013, 87, .	3.2	20
51	Influence of screening dynamics on excitons in Ga2O3 polymorphs. Applied Physics Letters, 2019, 114, .	3.3	20
52	Native defects and complexes in SiC. Journal of Physics Condensed Matter, 2001, 13, 9027-9037.	1.8	18
53	Carbon vacancy in SiC: A negative- U system. Europhysics Letters, 1998, 44, 309-314.	2.0	17
54	Polytypism and surface structure of SiC. Diamond and Related Materials, 1997, 6, 1346-1348.	3.9	16

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55	Efficient strain-induced light emission in lonsdaleite germanium. Physical Review Materials, 2021, 5, .	2.4	16
56	Intravacancy transition energies in3Câ^'and4Hâ^'SiC. Physical Review B, 2000, 61, 13655-13658.	3.2	15
57	Theory of atomic level magnetostrictive deformations and stresses in amorphous ferromagnets. Journal of Magnetism and Magnetic Materials, 1988, 75, 225-232.	2.3	14
58	Ab initiocalculation of optical properties with excitonic effects in wurtzite InxGa1â^'xN and InxAl1â^'xN alloys. Physical Review B, 2013, 87, .	3.2	14
59	Local magnetic anisotropy and magnetostriction of amorphous ferromagnets. Physica B: Condensed Matter, 1990, 161, 225-231.	2.7	13
60	Optical absorption and emission of Î±-Sn nanocrystals from first principles. Nanotechnology, 2013, 24, 405702.	2.6	13
61	Stoichiometry and surface reconstructions of (001) surfaces of silicon carbide. Surface Science, 1996, 352-354, 55-59.	1.9	12
62	Phase Separation, Gap Bowing, and Structural Properties of Cubic InxAl1â€"xN. Physica Status Solidi (B): Basic Research, 2002, 234, 956-960.	1.5	12
63	Band structure and electron gas of In chains on Si(111). Surface Science, 2005, 589, 77-90.	1.9	12
64	Various contributions to magnetostriction in amorphous and polycrystalline ferromagnets. Journal of Magnetism and Magnetic Materials, 1988, 72, 6-12.	2.3	11
65	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
66	Are amorphous ferromagnets with Î»S=0 magnetostrictive on a local scale?. Applied Physics Letters, 1991, 59, 2049-2051.	3.3	9
67	Electronic and Optical Properties of Small Metal Fluoride Clusters. ACS Omega, 2020, 5, 13268-13277.	3.5	8
68	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. Physical Review Materials, 2021, 5, .	2.4	7
69	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
70	Nonparabolicity and excitons in optical absorption of InN. Journal of Crystal Growth, 2006, 288, 294-297.	1.5	5
71	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. Physical Review B, 2011, 84, .	3.2	5
72	Dielectric and lattice-dynamical properties of III-nitrides. Journal of Electronic Materials, 2000, 29, 281-284.	2.2	4

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73	In4d and Ga3d levels in In_xX_{1â^'}_xN (Xâ€‰=â€‰Ga, Al) alloys. Applied Physics Letters, 2013, 102, 172105.	3.3	2
74	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
75	Towards a photonic band edge laser using hexagonal-SiGe nanowire arrays (Conference Presentation). , 2020, , .		1
76	INFLUENCE OF STRUCTURAL RELAXATION ON THE OPTICAL AND ELECTRONIC PROPERTIES OF Ge and Si NANOCRYSTALS. , 2005, , .		0