Jrgen Furthmller

List of Publications by Year in Descending Order

75 papers	45,694 citations	32 h-index	78 g-index
78 ext. papers	52,686 ext. citations	3.6 avg, IF	7.73 L-index

#	Paper	IF	Citations
75	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. *Physical Review Materials*, **2021**, 5,	3.2	2
74	Efficient strain-induced light emission in lonsdaleite germanium. *Physical Review Materials*, **2021**, 5,	3.2	5
73	Electronic and Optical Properties of Small Metal Fluoride Clusters. *ACS Omega*, **2020**, 5, 13268-13277	3.9	2
72	Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature*, **2020**, 580, 205-209	50.4	124
71	Influence of Polymorphism on the Electronic Structure of Ga2O3. *Chemistry of Materials*, **2020**, 32, 8460-8470	9.4	21
70	Influence of screening dynamics on excitons in Ga2O3 polymorphs. *Applied Physics Letters*, **2019**, 114, 122101	3.4	12
69	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. *Physical Review Materials*, **2019**, 3,	3.2	19
68	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. *Physical Review B*, **2019**, 100,	3.3	9
67	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. *Physical Review B*, **2016**, 94,	3.3	13
66	Dielectric tensor of monoclinic Ga2O3 single crystals in the spectral range 0.5–8.5 eV. *APL Materials* , **2015**, 3, 106106	5.7	65
65	One- and two-particle effects in the electronic and optical spectra of barium fluoride. *Journal of Physics Condensed Matter*, **2014**, 26, 125501	1.8	3
64	Structural and electronic properties of Sn□in nanocrystals from first principles. *Physical Review B*, **2013**, 87,	3.3	24
63	Electronic and optical properties of cadmium fluoride: The role of many-body effects. *Physical Review B*, **2013**, 87,	3.3	13
62	Ab initio calculation of optical properties with excitonic effects in wurtzite InxGa1−xN and InxAl1−xN alloys. *Physical Review B*, **2013**, 87,	3.3	13
61	Optical absorption and emission of Sn□n nanocrystals from first principles. *Nanotechnology*, **2013**, 24, 405702	3.4	10
60	In4d and Ga3d levels in InxX1−xN (X = Ga, Al) alloys. *Applied Physics Letters*, **2013**, 102, 172105	3.4	1
59	Electronic bands of III-V semiconductor polytypes and their alignment. *Physical Review B*, **2012**, 86,	3.3	126

58	Distribution of cations in wurtzitic InxGa1−xN and InxAl1−xN alloys: Consequences for energetics and quasiparticle electronic structures. *Physical Review B*, **2012**, 85,	3.3	18
57	GaMnAs: Position of Mn-d levels and majority spin band gap predicted from GGA-1/2 calculations. *Applied Physics Letters*, **2012**, 100, 202408	3.4	21
56	Electronic and optical properties of MgxZn1−xO and CdxZn1−xO fromab initiocalculations. *New Journal of Physics*, **2011**, 13, 085012	2.9	49
55	Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach. *Applied Physics Letters*, **2011**, 98, 151907	3.4	118
54	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. *Physical Review B*, **2011**, 84,	3.3	4
53	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,	3.3	57
52	Band-structure and optical-transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 2150-2153	1.3	56
51	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	33
50	Strain influence on valence-band ordering and excitons in ZnO: An ab initio study. *Applied Physics Letters*, **2007**, 91, 241915	3.4	52
49	Nonparabolicity and excitons in optical absorption of InN. *Journal of Crystal Growth*, **2006**, 288, 294-297	1.6	5
48	Magnetic properties of MnN: Influence of strain and crystal structure. *Applied Physics Letters*, **2005**, 86, 164105	3.4	25
47	Band structure and electron gas of In chains on Si(111). *Surface Science*, **2005**, 589, 77-90	1.8	12
46	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	1.3	20
45	Optical properties of Si and Ge nanocrystals: Parameter-free calculations. *Physica Status Solidi (B): Basic Research*, **2005**, 242, 3053-3063	1.3	30
44	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
43	Influence of oxygen on optical properties of Si nanocrystallites. *Applied Physics Letters*, **2005**, 87, 143113	3.4	24
42	Electron correlation effects on SiC(111) and SiC(0001) surfaces. *Journal of Physics Condensed Matter* , **2004**, 16, S1721-S1732	1.8	26
41	Energy gap and optical properties of InxGa1−xN. *Physica Status Solidi A*, **2003**, 195, 628-633		86

40	Lattice parameter and energy band gap of cubic AlxGayIn1−x−yN quaternary alloys. *Applied Physics Letters*, **2003**, 83, 890-892	3.4	65
39	Phase Separation, Gap Bowing, and Structural Properties of Cubic InxAl1−xN. *Physica Status Solidi (B): Basic Research*, **2002**, 234, 956-960	1.3	12
38	Do we know the fundamental energy gap of InN?. *Journal of Crystal Growth*, **2002**, 246, 315-319	1.6	112
37	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. *Applied Physics Letters*, **2002**, 80, 769-771	3.4	92
36	Gap bowing and Stokes shift in InxGa1−xN alloys: First-principles studies. *Applied Physics Letters*, **2002**, 80, 1394-1396	3.4	41
35	Spinodal decomposition in BxGa1−xN and BxAl1−xN alloys. *Applied Physics Letters*, **2002**, 80, 1177-1179	3.4	37
34	Phase diagram, chemical bonds, and gap bowing of cubic InxAl1−xN alloys: Ab initio calculations. *Journal of Applied Physics*, **2002**, 92, 7109-7113	2.5	31
33	Native defects and complexes in SiC. *Journal of Physics Condensed Matter*, **2001**, 13, 9027-9037	1.8	17
32	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	3.4	31
31	Dielectric and lattice-dynamical properties of III-nitrides. *Journal of Electronic Materials*, **2000**, 29, 281-284	1.9	4
30	First-principles calculations of the thermodynamic and structural properties of strained InxGa1−xN and AlxGa1−xN alloys. *Physical Review B*, **2000**, 62, 2475-2485	3.3	172
29	Intravacancy transition energies in 3C□ and 4H□SiC. *Physical Review B*, **2000**, 61, 13655-13658	3.3	14
28	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. *Physical Review B*, **2000**, 62, 6854-6857	3.3	57
27	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row and d-electron elements. *Physical Review B*, **2000**, 61, 4576-4587	3.3	98
26	Dynamics and polarization of group-III nitride lattices: A first-principles study. *Physical Review B*, **2000**, 62, 8003-8011	3.3	98
25	Initial stages of III-nitride growth. *Applied Physics Letters*, **1999**, 74, 3851-3853	3.4	20
24	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. *Physical Review B*, **1999**, 59, 15166-15180	3.3	211
23	Surface Energies and Surface Dipoles at III-Nitride(111) Surfaces in Dependence on Stoichiometry. *Physica Status Solidi (B): Basic Research*, **1999**, 216, 675-678	1.3	10

22	Polytypic transformations in SiC: An ab initio study. *Physical Review B*, **1999**, 60, 13261-13264	3.3	22
21	High-precision determination of atomic positions in crystals: The case of 6H- and 4H-SiC. *Physical Review B*, **1998**, 57, 2647-2650	3.3	93
20	Theoretical investigation of edge dislocations in AlN. *Applied Physics Letters*, **1998**, 72, 3467-3469	3.4	39
19	Si-rich SiC(111)/(0001)3□ and 3□ surfaces: A Mott-Hubbard picture. *Physical Review B*, **1998**, 58, 13712-13716	3.3	71
18	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. *Physical Review B*, **1998**, 58, R1722-R1725	3.3	64
17	Stacking faults in group-IV crystals: An ab initio study. *Physical Review B*, **1998**, 58, 1326-1330	3.3	78
16	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination of SiC(111)- (3□). *Physical Review Letters*, **1998**, 80, 758-761	7.4	162
15	Carbon vacancy in SiC: A negative- U system. *Europhysics Letters*, **1998**, 44, 309-314	1.6	17
14	Polytypism and surface structure of SiC. *Diamond and Related Materials*, **1997**, 6, 1346-1348	3.5	16
13	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. *Physical Review B*, **1997**, 56, 15629-15646	3.3	302
12	Structural and electronic properties of rhodium surfaces: an ab initio approach. *Surface Science*, **1996**, 346, 300-321	1.8	110
11	Stoichiometry and surface reconstructions of (001) surfaces of silicon carbide. *Surface Science*, **1996** , 352-354, 55-59	1.8	10
10	Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Computational Materials Science*, **1996**, 6, 15-50	3.2	41739
9	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. *Europhysics Letters*, **1995**, 32, 729-734	1.6	568
8	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. *Europhysics Letters*, **1994**, 28, 659-664	1.6	61
7	Are amorphous ferromagnets with □=0 magnetostrictive on a local scale?. *Applied Physics Letters*, **1991**, 59, 2049-2051	3.4	9
6	On the Change of Magnetostriction by Field Annealing of Amorphous Ferromagnetic Alloys. *Physica Status Solidi A*, **1990**, 117, K71-K75		6
5	Local magnetic anisotropy and magnetostriction of amorphous ferromagnets. *Physica B: Condensed Matter*, **1990**, 161, 225-231	2.8	12

4	Theory of atomic level magnetostrictive deformations and stresses in amorphous ferromagnets. *Journal of Magnetism and Magnetic Materials*, **1988**, 75, 225-232	2.8	14
3	Various contributions to magnetostriction in amorphous and polycrystalline ferromagnets. *Journal of Magnetism and Magnetic Materials*, **1988**, 72, 6-12	2.8	11
2	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. *Journal of Magnetism and Magnetic Materials*, **1987**, 69, 79-88	2.8	42
1	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. *Journal of Magnetism and Magnetic Materials*, **1987**, 69, 89-98	2.8	26